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General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, BioProcess ApS
Authors: Abeykoon Udugama, I. S. B. (Intern), Feldman, H. (Intern), Bryde-Jacobsen, J. (Ekstern), Gernaey, K. V. (Intern)
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Source-ID: 143952003
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Ab initio calculations and kinetic modeling of thermal conversion of methyl chloride: implications for gasification of biomass

Limitations in current hot gas cleaning methods for chlorine species from biomass gasification may be a challenge for end use such as gas turbines, engines, and fuel cells, all requiring very low levels of chlorine. During devolatilization of biomass, chlorine is released partly as methyl chloride. In the present work, the thermal conversion of CH₃Cl under gasification conditions was investigated. A detailed chemical kinetic model for pyrolysis and oxidation of methyl chloride was developed and validated against selected experimental data from the literature. Key reactions of CH₂Cl with O₂ and C₂H₄, for which data are scarce were studied by ab initio methods. The model was used to analyze the fate of methyl chloride in gasification processes. The results indicate that CH₃Cl emissions will be negligible for most gasification technologies, but could be a concern for fluidized bed gasifiers, in particular in low-temperature gasification. The present work illustrates how ab initio theory and chemical kinetic modeling can help to resolve emission issues for thermal processes in industrial scale.

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Web of Science (2012): Indexed yes
Web of Science (2011): Indexed yes
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
A fast and simple method to estimate relative, hyphal tensile-strength of filamentous fungi used to assess the effect of autophagy

Fungal hyphal strength is an important phenotype which can have a profound impact on bioprocess behavior. Until now, there is not an efficient method which allows its characterization. Currently available methods are very time consuming; thus, compromising their applicability in strain selection and process development. To overcome this issue, a method for fast and easy, statistically-verified quantification of relative hyphal tensile strength was developed. It involves off-line fragmentation in a high shear mixer followed by quantification of fragment size using laser diffraction. Particle size distribution (PSD) is determined, with analysis time on the order of minutes. Plots of PSD 90th percentile versus time allow estimation of the specific fragmentation rate. This novel method is demonstrated by estimating relative hyphal strength during growth in control conditions and rapamycin-induced autophagy for Aspergillus nidulans (paternal strain) and a mutant strain (∆Anatg8) lacking an essential autophagy gene. Both strains were grown in shake flasks, and relative hyphal tensile strength was compared. The mutant strain grown in control conditions appears to be weaker than the paternal strain, suggesting that Anatg8 may play a role in other processes involving cell wall biosynthesis. Furthermore, rapamycin-induced autophagy resulted in apparently weaker cells even for the mutant strain. These findings confirm the utility of the developed method in strain selection and process development.
Hyphal strength, Autophagy, Fermentation, Filamentous fungi, Fragmentation

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10.1002/bit.26490
A general overview of support materials for enzyme immobilization: Characteristics, properties, practical utility

In recent years, enzyme immobilization has been presented as a powerful tool for the improvement of enzyme properties such as stability and reusability. However, the type of support material used plays a crucial role in the immobilization process due to the strong effect of these materials on the properties of the produced catalytic system. A large variety of inorganic and organic as well as hybrid and composite materials may be used as stable and efficient supports for biocatalysts. This review provides a general overview of the characteristics and properties of the materials applied for enzyme immobilization. For the purposes of this literature study, support materials are divided into two main groups, called Classic and New materials. The review will be useful in selection of appropriate support materials with tailored properties for the production of highly effective biocatalytic systems for use in various processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Poznan University of Technology
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.44 SJR 0.928 SNIP 1.217
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.076 SNIP 1.246 CiteScore 3.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.683 SNIP 1.074 CiteScore 2.17
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.521 SNIP 0.582
Scopus rating (2012): SJR 0.471 SNIP 0.358
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Agglomeration mechanism in biomass fluidized bed combustion – Reaction between potassium carbonate and silica sand
Agglomeration is one of the operational problems in fluidized bed combustion of biomass, which is caused by interaction between bed materials (e.g. silica sand) and the biomass ash with a high content of potassium species. However, the contribution of different potassium species to agglomeration is not fully understood yet. In the present work, the reaction between K2CO3 and silica sand has been studied extensively by thermogravimetric analysis. The reacted samples were analyzed by SEM-EDX to reveal the reaction mechanism. The results indicated that the reaction occurs in a solid-solid phase already at temperatures around 700°C. The reaction rate increases with increasing temperature, but decreases with an increase of CO2 partial pressure. Using smaller particle size and well mixed solid reactants results in an increased reaction rate. It is observed that the reaction initiates in the contact area between K2CO3 and silica sand, forming a thin product layer. The layer acted as a reactive media further reacting with K2CO3 and silica sand. The results provide a
basis for understanding of potassium induced agglomeration process in fluidized bed biomass combustion.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST)
Authors: Anicic, B. (Intern), Lin, W. (Intern), Dam-Johansen, K. (Intern), Wu, H. (Intern)
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- Web of Science (2018): Indexed yes
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- Web of Science (2017): Indexed Yes
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- Scopus rating (2016): CiteScore 4.15 SJR 1.416 SNIP 1.722
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.519 SNIP 1.822 CiteScore 4.09
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.629 SNIP 2.161 CiteScore 3.96
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.636 SNIP 2.142 CiteScore 3.83
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.682 SNIP 2.075 CiteScore 3.77
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.575 SNIP 1.773 CiteScore 3.38
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.629 SNIP 1.88
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.545 SNIP 1.856
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.471 SNIP 1.718
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.226 SNIP 1.654
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 0.986 SNIP 1.404
- Scopus rating (2005): SJR 0.751 SNIP 1.143
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 0.82 SNIP 1.142
- Scopus rating (2003): SJR 0.941 SNIP 1.134
- Scopus rating (2002): SJR 0.731 SNIP 1.12
An exploratory study of three-dimensional MP-PIC-based simulation of bubbling fluidized beds with and without baffles

In this study, the flow characteristics of Geldart A particles in a bubbling fluidized bed with and without perforated plates were simulated by the multiphase particle-in-cell (MP-PIC)-based Eulerian-Lagrangian method. A modified structure-based drag model was developed based on our previous work. Other drag models including the Parker and Wen-Yu-Ergun drag models were also employed to investigate the effects of drag models on the simulation results. Although the modified structure-based drag model better predicts the gas-solid flow dynamics of a baffle-free bubbling fluidized bed in comparison with the experimental data, none of these drag models predict the gas-solid flow in a baffled bubbling fluidized bed sufficiently well because of the treatment of baffles in the Barracuda software. To improve the simulation accuracy, future versions of Barracuda should address the challenges of incorporating the bed height and the baffles.
A probabilistic model-based soft sensor to monitor lactic acid bacteria fermentations

A probabilistic soft sensor based on a mechanistic model was designed to monitor *S. thermophilus* fermentations, and validated with experimental lab-scale data. It considered uncertainties in the initial conditions, on-line measurements, and model parameters by performing Monte Carlo simulations within the monitoring system. It predicted, therefore, the probability distributions of the unmeasured states, such as biomass, lactose, and lactic acid concentrations. To this end, a mechanistic model was developed first, and a statistical parameter estimation was performed in order to assess parameter sensitivities and uncertainties. The model coupled a biokinetic and a mixed weak acid/base model to predict biological variables and chemical variables like the pH, respectively. In the soft sensor, the limited available on-line measurements, namely the quantity of added ammonia and pH, were used to update the model parameters that were then used as input to the mechanistic model. The soft sensor predicted both the current state variables, as well as the future course of the fermentation, e.g. with a relative mean error of the biomass concentration of 8 %. This successful implementation of a process analytical technology monitoring system opens up further opportunities, including for on-line risk-based monitoring and control applications.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, PILOT PLANT, Chr. Hansen AS
Authors: Spann, R. (Intern), Roca, C. (Ekstern), Kold, D. (Ekstern), Eliasson Lantz, A. (Intern), Gernaey, K. V. (Intern), Sin, G. (Intern)
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.75
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.15
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.95
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
A thermo-reversible silicone elastomer with remotely controlled self-healing

Soft thermoplastic elastomers with increased durability and reliability are in high demand for a broad spectrum of applications. Silicone elastomers are soft and durable, but they are not thermoplastic in nature, and under extreme conditions such as high voltage or large deformations, reliability may also suffer. Thus, as a solution to these shortcomings, which are typical of silicone elastomers, it is natural to propose a thermo-reversible, self-healing, and recyclable silicone-based elastomer. Stimuli-responsivity is imparted to the silicone polymer by incorporating supramolecular 2-ureido-4\([1H]\)-pyrimidone (UPy) self-assembling motifs via free radical polymerisation. Self-healing of the novel elastomer may be triggered by both direct and indirect heating, the latter by means of incorporating Fe\(_3\)O\(_4\) particles into the elastomer and subsequent exposure to an alternating magnetic field. As a consequence of temperature responsiveness and high thermal stability, the elastomer is proven recyclable, by withstanding multiple reprocessing procedures with no substantial effects on the resulting properties. The synergy of these valuable characteristics makes this novel material a smart candidate for innumerable applications where soft and reliable elastomers are sought.
A Water Treatment Case Study for Quantifying Model Performance with Multilevel Flow Modelling

Decision support systems are a key focus of research on developing control rooms to aid operators in making reliable decisions, and reducing incidents caused by human errors. For this purpose, models of complex systems can be developed to diagnose causes or consequences for specific alarms. Models applied in safety systems of complex and safety-critical systems require rigorous and reliable model building and testing. Multilevel Flow Modelling is a qualitative and discrete method for diagnosing faults and has previously only been validated by subjective and qualitative means. To ensure reliability during operation, this work aims to synthesize a procedure to measure model performance according to diagnostic requirements. A simple procedure is proposed for validating and evaluating the concept of Multilevel Flow Modelling. For this purpose, expert statements, dynamic process simulations, and pilot plant experiments are used for validation of simple Multilevel Flow Modelling models of a hydrocyclone unit for oil removal from produced water.
Biocatalyst Screening with a Twist: Application of Oxygen Sensors Integrated in Microchannels for Screening Whole Cell Biocatalyst Variants

Selective oxidative functionalization of molecules is a highly relevant and often demanding reaction in organic chemistry. The use of biocatalysts allows the stereo- and regioselective introduction of oxygen molecules in organic compounds at milder conditions and avoids the use of complex group-protection schemes and toxic compounds usually applied in conventional organic chemistry. The identification of enzymes with the adequate properties for the target reaction and/or substrate requires better and faster screening strategies. In this manuscript, a microchannel with integrated oxygen sensors was applied to the screening of wild-type and site-directed mutated variants of naphthalene dioxygenase (NDO) from Pseudomonas sp. NICB 9816-4. The oxygen sensors were used to measure the oxygen consumption rate of several variants during the conversion of styrene to 1-phenylethanediol. The oxygen consumption rate allowed the distinguishing of endogenous respiration of the cell host from the oxygen consumed in the reaction. Furthermore, it was possible to identify the higher activity and different reaction rate of two variants, relative to the wild-type NDO. The meander microchannel with integrated oxygen sensors can therefore be used as a simple and fast screening platform for the selection of dioxygenase mutants, in terms of their ability to convert styrene, and potentially in terms of substrate specificity.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Universität Stuttgart
Authors: Fernandes, A. C. (Intern), Halder, J. M. (Ekstern), Nestl, B. M. (Ekstern), Hauer, B. (Ekstern), Gernaey, K. V. (Intern), Krühne, U. (Intern)
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Whole cell biocatalysis, Biocatalyst screening; Microfluidics, Oxygen sensors, Dioxygenases, Organic chemistry
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CFD modelling of axial mixing in the intermediate and final rinses of cleaning-in-place procedures of straight pipes
The intermediate and final rinses of straight pipes, in which water replaces a cleaning agent of similar density and viscosity, are modelled using Computational Fluid Dynamic (CFD) methods. It is anticipated that the displacement process is achieved by convective and diffusive transport. The simulated agent concentrations show good agreement with the analytical axial mixing models from literature. The displacement time, minimum water consumption, minimum generation of wastewater and minimum requirement of intermediate rinsing water are evaluated using CFD. Practical empirical equations are derived from CFD results and applied to examine if the process is operated in an efficient and economic manner. It has been found that the displacement time can be predicted from the inner pipe diameter and the mean flow
velocity using a power law relationship. Changing flow velocities does not significantly influence the minimum water consumption and the minimum wastewater generation for rinsing a pipe. Controlling the rinsing step based on a downstream measurement still consumes more water than the minimum requirement to reduce contamination risks. This article presents an innovative algorithm for optimizing the rinse steps with lower water consumption based on the above observations. A case of rinsing a 24 m long straight pipe describes the promising application of the CFD study. The recovery of cleaning agent can be up to 89.3% of the volume and the saving of intermediate rinsing water can be at least 55% compared to the conventional rinse method. The work in this article presents an example showing how to deal with more complex systems in the future.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Alfa Laval, Alfa Laval, Carlsberg
Authors: Yang, J. (Intern), Jensen, B. B. B. (Ekstern), Nordkvist, M. (Ekstern), Rasmussen, P. (Ekstern), Gernaey, K. V. (Intern), Krühne, U. (Intern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.71 SJR 1.479 SNIP 1.842
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.467 SNIP 1.873 CiteScore 3.58
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.524 SNIP 1.975 CiteScore 3.44
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.348 SNIP 1.908 CiteScore 3.1
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.394 SNIP 1.993 CiteScore 2.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.329 SNIP 1.922 CiteScore 2.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.439 SNIP 1.793
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.411 SNIP 1.623
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.301 SNIP 1.521
Scopus rating (2007): SJR 1.044 SNIP 1.958
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.101 SNIP 1.546
CO2 Mass transfer model for carbonic anhydrase-enhanced aqueous MDEA solutions

In this study a CO2 mass transfer model was developed for carbonic anhydrase-enhanced MDEA solutions based on a mechanistic kinetic enzyme model. Four different enzyme models were compared in their ability to predict the liquid side mass transfer coefficient at temperatures in the range of 298 to 328 K, solvent concentrations in the range 15 to 50 wt%, CO2 partial pressures up to 50 kPa, solvent loading between 0 and 0.5 mole CO2 per mole MDEA and enzyme concentrations up to 8.5 g/L. The reversible Michaelis Menten model (MR) and the simplified model with product inhibition by the bicarbonate ion (SP) were able to predict the mass transfer with an absolute average relative deviation of less than 15%. The MR model could account for every influence (solvent concentration, temperature, solvent loading, CO2 partial pressure) of the different process conditions on the mass transfer, whereas the SP model is limited to applications with low CO2 partial pressure such as CCS from coal burning power plants. Two other models that were also investigated are not suitable for implementation into an absorber column simulation, as they cannot describe the influence of changing solvent loading on the mass transfer.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.34
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Cobalt/N-Hydroxyphthalimide(NHPI)-Catalyzed Aerobic Oxidation of Hydrocarbons with Ionic Liquid Additive

A highly efficient and solvent-free system of cobalt/NHPI-catalyzed aerobic oxidation of hydrocarbons was developed using imidazolium-based ionic liquid (IL) as an additive. These amphipathic ILs were found self-assemble at the interface between the organic hydrocarbons and the aqueous phase of catalyst combination (Co/NHPI), with forming a solution of reversed multilamellar vesicles for catalysis. The initial reaction rate was influenced by both the composition of microdomains and the structure of IL launched. Consequently, a proper water content (XH2O) of wet IL was requisite to reach the optimum reactivity. Besides, the interfacial boundary between aqueous and organic phase composed by C2-alkylated imidazolium ILs, such as [bdmim]SbF6 and [C12dmim]SbF6, not only has ternary aggregates (hydrocarbons/IL/H2O) of higher stability but renders O2 a faster diffusion rate and higher concentration, thereby offering a high reactivity of the protocol towards hydrocarbon oxidation.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Chinese Academy of Sciences
Authors: Mahmood, S. (Ekstern), Xu, B. H. (Ekstern), Ren, T. L. (Ekstern), Zhang, Z. (Intern), Liu, X. (Ekstern), Zhang, S. (Ekstern)
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Source: FindIt
Source-ID: 2396389781
Combined polyhydroxyalkanoates (PHA) and 1,3-propanediol production from crude glycerol: Selective conversion of volatile fatty acids into PHA by mixed microbial consortia

Crude glycerol is an important by-product of the biodiesel industry, which can be converted into volatile fatty acids (VFA) and/or 1,3-propanediol (1,3-PDO) by fermentation. In this study, a selective conversion of VFA to polyhydroxyalkanoates (PHA) was attained while leaving 1,3-PDO in the supernatant by means of mixed microbial consortia selection strategies. The process showed highly reproducible results in terms of PHA yield, 0.99 ± 0.07 Cmol PHA/Cmol S (0.84 g COD PHA/g COD S), PHA content (76 ± 3.1 g PHA/100 g TSS) and 1,3-PDO recovery (99 ± 2.1%). The combined process had an ultimate yield from crude glycerol of 0.19 g COD PHA and 0.42 g COD 1,3-PDO per g of input COD. The novel enrichment strategy applied for selectively transforming fermentation by-products into a high value product (PHA) demonstrates the significance of the enrichment process for targeting specific bio-transformations and could potentially prove valuable for other biotechnological applications as well.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, The Danish Polymer Centre, PILOT PLANT, SINTEF
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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.49 SJR 2.629 SNIP 2.558
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.689 SNIP 2.507 CiteScore 6.63
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.957 SNIP 2.727 CiteScore 6.13
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.956 SNIP 2.693 CiteScore 6.02
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.966 SNIP 2.456 CiteScore 5.15
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.867 SNIP 2.374 CiteScore 5.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.582 SNIP 2.196
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Compared leaf anatomy and water relations of commercial and traditional Prunus dulcis (Mill.) cultivars under rain-fed conditions

Leaf anatomy and water relations of seven almond (Prunus dulcis Mill.) cultivars, traditional (Bonita, Casanova, Parada, Pegarinhos and Verdeal) and commercial (Ferragnès and Glorieta), grown under rain-fed conditions, were studied. The performed measurements included thickness of leaf tissues, leaf area, leaf mass per unit area, density of leaf tissue, relative water content, succulence, water saturation deficit, water content at saturation and cuticular transpiration rate. Significant differences were observed in most of the studied parameters between cultivars. Overall results indicate that traditional cultivars Bonita, Casanova and Pegarinhos have developed more morphological and structural leaf adaptations to protect against water loss than the other cultivars. If Bonita cultivar relies on reduced leaf area and stomatal density, thicker cell wall and leaf density, Casanova has increased cuticle thickness, while Pegarinhos adds a thicker epidermis and palisade parenchyma to increase protection to water loss. These data is one of the first comparative approaches to the leaf characterization of these cultivars, and should now be combined with physiological and biochemical studies, to further elucidate the adaptation processes of almond cultivars to harmful environments.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Universidade de Tras-os-Montes e Alto Douro
Authors: Oliveira, I. (Ekstern), Meyer, A. (Intern), Afonso, S. (Ekstern), Gonçalves, B. (Ekstern)
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Despite numerous reports regarding the potential of graphene for corrosion protection, examples of chemical vapor deposited (CVD) graphene-based anticorrosive coatings able to provide long-term protection (i.e., several months) of metals have so far been absent. Here, we present a polymer-graphene hybrid coating, comprising two single layers of CVD graphene sandwiched by three layers of polyvinyl butyral, which provides complete corrosion protection of commercial aluminum alloys even after 120 days of exposure to simulated seawater. The essential role played by graphene in the hybrid coating is evident when we compare the results from a polymer-only coating of the same thickness, which fails in protecting the metal after less than 30 days. With the emergence of commercially available large-area CVD graphene, our work demonstrates a straightforward approach towards high-performance anticorrosive coatings, which can be extended to other two-dimensional materials and polymers, for long-term protection of various relevant metals and alloys.
Science and Technology Centre (CoaST), University of Manchester
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 6.49 SJR 2.077 SNIP 1.666
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.042 SNIP 1.756 CiteScore 6.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.145 SNIP 2.014 CiteScore 6.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.292 SNIP 2.137 CiteScore 6.54
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.525 SNIP 2.135 CiteScore 5.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.174 SNIP 2.073 CiteScore 5.23
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.404 SNIP 2.055
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.132 SNIP 2.119
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.128 SNIP 1.96
Scopus rating (2007): SJR 1.845 SNIP 1.828
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.786 SNIP 1.862
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.426 SNIP 1.699
Scopus rating (2004): SJR 1.514 SNIP 1.906
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.595 SNIP 1.749
Scopus rating (2002): SJR 1.775 SNIP 1.813
Scopus rating (2001): SJR 1.304 SNIP 1.433
Scopus rating (2000): SJR 1.032 SNIP 1.342
Configuration optimization of series flow double-effect water-lithium bromide absorption refrigeration systems by cost minimization

An optimal process configuration for double-effect water-lithium bromide absorption refrigeration systems with series flow – where the solution is first passed through the high-temperature generator – is obtained by minimization of the total annual cost for a required cooling capacity. To this end, a nonlinear mathematical programming approach is used. Compared to the optimized conventional double-effect configuration, the new optimal configuration obtained in this paper allows reducing the total annual cost, the capital expenditures, and the operating expenditures by around 9.5%, 11.1% and 4.9%, respectively. Most importantly, the obtained optimal solution eliminates the low-temperature solution heat exchanger from the conventional configuration, rendering a new process configuration. The energy integration between the weak and strong lithium bromide solutions (cold and hot streams, respectively) takes place entirely at the high-temperature zone, and the sizes and operating conditions of the other process units change accordingly in order to meet the problem specification with the minimal total annual cost. This new configuration was obtained for wide ranges of the cooling capacity (150–450kW) and the temperature of the cooling water (15–35°C). The results of this work motivate to apply the simultaneous optimization approach to seek for new multi-effect absorption refrigeration system configurations with parallel and reverse flow as well as other series flow arrangements that minimize the total annual cost.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, CONICET, Technische Universität Berlin
Authors: Mussati, S. F. (Ekstern), Cignitti, S. (Intern), Mansouri, S. S. (Intern), Gernaey, K. V. (Intern), Morosuk, T. (Ekstern), Mussati, M. C. (Ekstern)
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 6.04 SJR 2.287 SNIP 2.065
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.09 SNIP 2.092 CiteScore 5.24
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.854 SNIP 2.835 CiteScore 5.35
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.669 SNIP 2.558 CiteScore 4.49
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 2.277 CiteScore 3.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Corrigendum to "Rheological properties of agar and carrageenan from Ghanaian red seaweeds" [Food Hydrocolloids 63 (2017) 50–58]

The authors regret that the <data published in Table 3> in the paper report slightly too high values for the 3,6-anhydrogalactose, which in some cases infer that the level of anhydro-galactose is higher than the level of galactose in the hydrocolloids. This is in fact not correct. The corrected data differ by only 1–3% from the ones published, but show that in no case is the anhydro-galactose level higher than the level of galactose in the hydrocolloids. The 3,6-anhydro-galactopyranosyl moieties were initially determined by HPAEC-PAD using a CarboPac™ PA20 column following the reducing acid hydrolysis using TFA and MMB, as described by Jol et al. (1999). The procedure for the reducing acid hydrolysis includes three additions of the reducing agent MMB. To improve the subsequent HPAEC-PAD quantification, the third addition of MMB was initially left out, as it resulted in better retention and resolution in the HPAEC-PAD quantification. The experiments have since been repeated following the exact procedure for the reducing acid hydrolysis (Jol et al., 1999). Carbohydrate compositions have been determined using the CarboPac™ PA1 column with accompanying guard column. Elution was performed using 500 mM NaOH and an isotropic flow on 0.4 mL/min. Quantification was performed with glucose, galactose, and 3,6-anhydro-galactose as sugar standards that had been reduced by the reductive acid hydrolysis as well. The new data are presented in the corrected Table 3 below. Reference: Jol, C. N., Neiss, T. G., Penninkhof, B., Rudolph, B., & De Ruiter, G. A. (1999). A novel high-performance anion-exchange chromatographic method for the analysis of carrageenans and agars containing 3,6-anhydrogalactose. Analytical Biochemistry, 268, 213-222. Table 3 Overview of seaweed type (hydrocolloid source), hydrocolloid extraction method (direct water-extraction or after alkali treatment), hydrocolloid and monomer1 yields, and sulfate levels [data given as means±SD]. Different roman superscript letters indicate significant differences (P<0.05) column-wise for carrageenans and agar yields, monosaccharides, and sulfate content by one-way ANOVA.
Design and preliminary operation of a hybrid syngas/solar PV/battery power system for off-grid applications: A case study in Thailand

Due to the irregular nature of solar resource, solar photovoltaic (PV) system alone cannot satisfy load on a 24/7 demand basis, especially with increasing regional population in developing countries such as Thailand. A hybrid solar PV/biomass based along with battery storage system has been drawing more attention to option since it promises great deal of challenges and opportunities for different rural areas. Thailand rich with higher level of agricultural crops and biomass materials, is a prospective candidate for deployment of bio-power to complement such hybrid systems. To this end, in this study a customized hybrid power system integrating solar, biomass (syngas) power and battery storage system is evaluated a pilot scale for micro off-grid application. This paper shows that for a reliability of a hybrid syngas/solar PV system along with rechargeable batteries, the syngas generator can guarantee a continuous 24 hours electricity supply in case of shortage of energy (during on cloudy day and at the nighttime). Two consecutive days of commissioning phase are necessary for the entire system to operate, which is a solid basis for including the syngas generator in the hybrid system. Furthermore, the generator has to be always synchronized during the commissioning time. Battery state of charge (SOC) in percent (%) connecting with syngas is greater than solar PV and the charging time appears significantly shorter than that one. All possible combinations between an innovation and existing systems can serve as a guideline for making similar studies in the context of different off-grid sites and more. Next, optimal scale up and design of hybrid power system for different off grid applications will be performed including comprehensive uncertainty analysis to facilitate robust and renewable electricity generation.

General information
State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, King Mongkut's University of Technology North Bangkok
Authors: Kohsri, S. (Ekstern), Meechai, A. (Ekstern), Prapainainar, C. (Ekstern), Narataraksa, P. (Ekstern), Hunpinyo, P. (Ekstern), Sin, G. (Intern)
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BFI (2018): BFI-level 2
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.855 SNIP 1.449 CiteScore 2.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.957 SNIP 1.668 CiteScore 2.56
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.912 SNIP 1.335 CiteScore 2.12
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Developing a framework to model the primary drying step of a continuous freeze-drying process based on infrared radiation

The continuous freeze-drying concept based on spinning the vials during freezing and on non-contact energy transfer via infrared (IR) radiation during drying, improves process efficiency and product quality (uniformity) compared to conventional batch freeze-drying. Automated control of this process requires the fundamental mechanistic modelling of each individual process step. Therefore, a framework is presented for the modelling and control of the continuous primary drying step based on non-contact IR radiation. The IR radiation emitted by the radiator filaments passes through various materials before finally reaching the spin frozen vial. The energy transfer was computed by combining physical laws with Monte Carlo simulations and was verified with experimental data. The influence of the transmission properties of various materials on the emitted IR radiation profile was evaluated. These results assist in the selection of proper materials which could serve as IR window in the continuous freeze-drying prototype. The modelling framework presented in this paper fits the model-based design approach used for the development of this prototype and shows the potential benefits of this design strategy by establishing the desired engineering parameters and by enabling the engineer to assess mechanical tolerances and material options.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Ghent University
Authors: Van Bockstal, P. (Ekstern), Corver, J. (Ekstern), Mortier, S. T. F. (Ekstern), De Meyer, L. (Ekstern), Nopens, I. (Ekstern), Gernaey, K. V. (Intern), De Beer, T. (Ekstern)
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Directing filtration to narrow molecular weight distribution of oligodextran in an enzymatic membrane reactor

Oligodextrans with molecular weight (Mw) within the range of 5.0–8.0kDa have great commercial potential as precursors of iron-dextran for anemia treatment. Traditional oligodextran production consists of sucrose fermentation, acid hydrolysis and ethanol precipitation, which results in an uneven Mw product, hypersaline wastewater discharge and potential safety hazards. In this work, a novel enzymatic membrane reactor (EMR) system to produce oligodextran is proposed, whereby in-situ product recovery can be manipulated to control the Mw distribution of the resulting products. Results showed that the membrane material played an important role in the permeate flux and transmission of oligodextran. Among the tested membranes, a 20kDa polyethersulfone (PES) membrane was found to be optimal for building up the EMR, as it
successfully controlled the oligodextran Mw within the desired range with a relatively narrow distribution and high productivity. Moreover, high transmembrane pressures (3 bars) and low stirring rates (160rpm) promoted yields beyond 50% in 120min. Higher permeate fluxes prevented further product hydrolysis and enhanced the yield. However, the resulting concentration polarization (CP) should be minimized to reduce accumulation of large oligodextran molecules on the membrane surface, which might diffuse through the membrane and thus broaden the Mw distribution of the products in the permeate. Both dextranase and dextran caused membrane irreversible fouling. The fouling caused by the enzymes not only favored the enzyme immobilization itself, but also contributed to narrow the membrane pore size distribution. As a result, a higher uniformity of oligodextran products compared with the pristine EMR was obtained, especially at the beginning of operation with EMR (which was improved by 22%). It was concluded that selecting the suitable membrane type and permeate flux, maximizing the shear rate, and narrowing the membrane pore size distribution were effective strategies to obtain high-quality oligodextran products by EMRs.

General information
State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Chinese Academy of Sciences
Authors: Su, Z. (Ekstern), Luo, J. (Ekstern), Pinelo, M. (Intern), Wan, Y. (Ekstern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.062 SNIP 1.72
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2 SNIP 1.771 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.433 SNIP 1.935 CiteScore 5.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.452 SNIP 2.001 CiteScore 5.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.201 SNIP 1.968 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.82 SNIP 1.726 CiteScore 4.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.821
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.638 SNIP 1.693
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.461 SNIP 1.805
Distribution and occurrence of lithium in high-alumina-coal fly ash

High-alumina-coal fly ash (HAFA) with a high Li content is regarded as a potential resource for Li production. To support the development of Li recovery technology from HAFA, the distribution and modes of occurrence of Li in HAFA were investigated. HAFA was separated into magnetic particles, glass, and mullite+corundum+quartz (MCQ) using an acid-alkali combination method. 79–94% of the Li was found in glass, with the remaining 5–16% and <5% of Li in MCQ and magnetic particles, respectively. Chemical state imaging of Li in HAFA, magnetic particles, and MCQ was obtained using time-of-flight secondary ion mass spectrometry (TOF-SIMS). Lithium was found to be relatively uniformly distributed in the HAFA particles and strongly correlated with Al and Si. Possible formation pathways of Li in the glass phase were proposed. The energy differences between reactants and products (∆E) calculated using the generalized gradient approximation (GGA) method indicated that Li occurred in Q3(0Al) and Q3(1Al) structures by reacting with Q4(0Al) and Q4(1Al). Based on the experimental and simulation results, we propose extracting Li during the pre-desilication process by dissolving the glass phase.
Drag resistance of ship hulls: Effects of surface roughness of newly applied fouling control coatings, coating water absorption, and welding seams

Fouling control coatings (FCCs) and irregularities (e.g., welding seams) on ship hull surfaces have significant effects on the overall drag performance of ships. In this work, skin frictions of four newly applied FCCs were compared using a pilot-scale rotary setup. Particular attention was given to the effects of coating water absorption on skin friction. Furthermore, to investigate the effects of welding seam height and density (number of welding seams per five meters of ship side) on drag resistance, a new flexible rotor was designed and used for experimentation.

It was found, under the conditions selected, that a so-called fouling release (FR) coating caused approximately 5.6% less skin friction (torque) over time than traditional biocide-based antifouling (AF) coatings at a tangential speed of 12 knots. Furthermore, results of immersion experiments and supporting "standard" water absorption experiments showed that water absorption of the FR coating did not result in any significant impacts on skin friction. On the other hand, water absorption was found to actually lower the skin friction of AF coatings. This may be attributed to a smoothening of the coating surface.

The effects of welding seam height and density on drag resistance were found to be substantial when welding seam height is above 5 mm, especially at high tangential speeds (above 15 knots). Using an interpolation approach, the pilot-scale welding seam drag data could be used to estimate the drag resistance at approximated full-scale conditions, equivalent to about one welding seam per five meters of ship side. It was shown, in this case, that the contribution of welding seams to ship skin friction could very well be less significant than those of FCCs when the welding seam height is below 5 mm, a representative value for full-scale welding seam height.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Hempel AS, Hempel, Maersk Line
Authors: Wang, X. (Intern), Olsen, S. M. (Ekstern), Andrés, E. (Ekstern), Kiil, S. (Intern), Olsen, K. N. (Ekstern)
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.44 SJR 0.409 SNIP 0.614
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.45 SJR 0.421 SNIP 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Efficient One-Step Fusion PCR Based on Dual-Asymmetric Primers and Two-Step Annealing

Gene splicing by fusion PCR is a versatile and widely used methodology, especially in synthetic biology. We here describe a rapid method for splicing two fragments by one-round fusion PCR with a dual-asymmetric primers and two-step annealing (ODT) method. During the process, the asymmetric intermediate fragments were generated in the early stage. Thereafter, they were hybridized in the subsequent cycles to serve as template for the target full-length product. The process parameters such as primer ratio, elongation temperature and cycle numbers were optimized. In addition, the fusion products produced with this method were successfully applied in seamless genome editing. The fusion of two fragments by this method takes less than 0.5 day. The method is expected to facilitate various kinds of complex genetic engineering projects with enhanced efficiency.

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, University of Nebraska, Chinese Academy of Sciences
Authors: Liu, Y. (Ekstern), Chen, J. (Ekstern), Thygesen, A. (Intern)
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Web of Science (2017): Indexed Yes
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Elasticity and electrical resistivity of chalk and greensand during water flooding with selective ions

Water flooding with selective ions has in some cases lead to increased oil recovery. We investigate the physical processes on a pore scale that are responsible for changes in petrophysical and mechanical properties of four oil-bearing chalk and four oil-bearing greensand samples caused by flooding with brines containing varying amounts of dissolved NaCl, Na₂SO₄, MgCl₂ and MgSO₄. Ultrasonic P-wave velocity and AC resistivity measurements were performed prior to, during and after flow through experiments in order to identify and quantify the processes related to water flooding with selective ions. Low field Nuclear Magnetic Resonance (NMR) spectrometry measurements were performed at full water saturation, at irreducible water saturation, after aging and after flooding. CT-scanning, X-ray diffraction (XRD), backscatter electron microscopy images (BSEM), mercury injection capillary pressure (MICP) curves and specific surface analysis (BET) reveal the mineralogy and texture of the rock samples before and after the injection. Low field NMR data indicates changes in the pore fluid distribution and wettability of chalk after aging of one of the samples. NMR data for other samples indicate that chalk is water-wet after flooding. Greensand remained mixed wet throughout the experiments. Electrical resistivity data are in agreement with this interpretation. The electrical resistivity data during flooding revealed that the formation brine is not fully replaced by the injected water in both chalk and greensand. Changes in the elasticity of chalk during flooding illustrate the softening effect of magnesium bearing brines as compared to the sodium bearing brines. The stiffness of greensand was not affected by water flooding with selective ions as determined from the elastic wave measurements. Precipitation of fines during flooding of chalk samples is indicated by an increase in specific surface area and a shift in the MICP to lower values but no fines were detected by NMR. No changes were observed for greensand samples.
Enzyme activities at different stages of plant biomass decomposition in three species of fungus-growing termites

Fungus-growing termites rely on the mutualistic fungus Termitomyces and gut microbes for plant biomass degradation. Due to a certain degree of symbiont complementarity, this tripartite symbiosis has evolved as a complex bioreactor, enabling decomposition of nearly any plant polymer, likely contributing to the success of the termites as the main plant decomposers in the Old World. Here we evaluate which plant polymers are decomposed and which enzymes are active during the decomposition process in two major genera of fungus-growing termites. We find a diversity of active enzymes at different stages of decomposition and a consistent decrease in plant components during the decomposition process. Furthermore, our findings are consistent with the hypothesis that termites transport enzymes from the older mature parts of the fungus comb through young worker guts to freshly inoculated plant substrate. However, preliminary fungal RNAseq analyses suggest that this likely transport is supplemented with enzymes produced in situ. Our findings support that the maintenance of an external fungus comb, inoculated with an optimal mix of plant material, fungal spores, and enzymes, is likely the key to the extraordinarily efficient plant decomposition in fungus-growing termites. Importance: Fungus-growing termites have a substantial ecological footprint in the old world (sub)tropics due to their ability to decompose dead plant material. Through the establishment of an elaborate plant biomass inoculation strategy, and fungal and bacterial enzyme contributions, this farming symbiosis has become an efficient and versatile aerobic bioreactor for plant substrate conversion. Since little is known about what enzymes are expressed, and where they are active at different stages of the decomposition process, we used enzyme assays, transcriptomics and plant content measurements to shed light on how this decomposition of plant substrate is effectively accomplished.

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.08
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Estimation of Physical Properties of Amino Acids by Group- Contribution Method

In this paper, we present group-contribution (GC) based property models for estimation of physical properties of amino acids using their molecular structural information. The physical properties modelled in this work are normal melting point
(T_m), aqueous solubility (W_s), and octanol/water partition coefficient (K_{ow}) of amino acids. The developed GC-models are based on the published GC-method by Marrero and Gani (J. Marrero, R. Gani, Fluid Phase Equilib. 2001, 183-184, 183-208) with inclusion of new structural parameters (groups and molecular weight of compounds). The main objective of introducing these new structural parameters in the GC-model is to provide additional structural information for amino acids having large and complex structures and thereby improve predictions of physical properties of amino acids. The group-contribution values were calculated by regression analysis using a data-set of 239 values for T_m, 211 values for W_s, and 335 values for K_{ow}. Compared to other currently used GC-models, the developed models make significant improvements in accuracy with average absolute error of 10.8 K for T_m and logarithm-unit average absolute errors of 0.16 for K_{ow} and 0.19 for W_s.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CERE – Center for Energy Ressources Engineering, Alfa Laval
Authors: Jhamb, S. V. (Intern), Liang, X. (Intern), Gani, R. (Intern), Hukkerikar, A. S. (Ekstern)
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.319 SNIP 1.708
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.293 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.299 SNIP 1.6
Web of Science (2008): Indexed yes
Over the last few decades, ion exchange membranes have evolved from a laboratory tool to industrial products with significant technical and commercial impacts. Electrodialysis with bipolar membranes (EDBM) is a technology that can produce acids and bases from the corresponding salt solutions. Bipolar membranes are key factors for splitting water at the interface of a cation and anion exchange layer in an electric field. The ideal bipolar membrane should have a low energy consumption, a high current efficiency and long-term stability. In order to investigate the catalytic effect of a monolayer of MoS2, the bipolar membranes were prepared by introducing monolayer MoS2 to the interface of bipolar membranes. The resulting bipolar membrane was found to have lower potential drop, which clearly demonstrates the applicability of the MoS2 layer to act as catalyst. Enhanced acid production confirmed this prediction. Furthermore, a bipolar membrane prepared at 90°C had a low swelling ratio of about 7.5% while maintaining a high water uptake of 71.6%. From the calculation of current efficiency and energy consumption, the bipolar membrane with a monolayer of MoS2 has a higher current efficiency (45%) and a lower energy consumption (3.6 kW·h/kg) compared to a current efficiency of 24% and an energy consumption of 6.3 kW·h/kg for a bipolar membrane without MoS2. This study proves the catalytic function of MoS2, which lays a foundation for further research on catalytic bipolar exchange membranes.

Exfoliated MoS2 nanosheets loaded on bipolar exchange membranes interfaces as advanced catalysts for water dissociation

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, KU Leuven, Fuzhou University, Zhejiang University of Technology
Authors: Li, J. (Ekstern), Morthensen, S. T. (Intern), Zhu, J. (Ekstern), Yuan, S. (Ekstern), Wang, J. (Ekstern), Volodine, A. (Ekstern), Lin, J. (Ekstern), Shen, J. (Ekstern), Van der Bruggen, B. (Ekstern)
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.023 SNIP 1.394
Experimental data of the aqueous NH$_3$ and CO$_2$ absorption at temperatures from 15 °C to 35 °C, NH$_3$ concentrations from 5% to 15% and CO$_2$ loadings from 0.2 to 0.6 measured with the Wetted Wall Column

The absorption between aqueous NH$_3$ and CO$_2$ is studied using the Wetted Wall Column in order to show the effect of the solvent condition on the rate of reaction. A total of 27 different cases are investigated in the region defined by temperatures from 15°C to 35°C, NH$_3$ concentrations from 5% to 15% and CO$_2$ loadings from 0.2 to 0.6. The paper reports the data measured during the experiments, the experimental apparatus description and the experimental procedure. The data here presented are both the raw data measured with their uncertainty and the final value of the overall mass transfer coefficient. The overall mass transfer coefficient is the result of the raw data treatment explained in the research paper related to this data. The data here reported are analyzed in the paper by Lillia et al. (2018) [1].
Experimental study of the aqueous CO2-NH3 rate of reaction for temperatures from 15°C to 35°C, NH3 concentrations from 5% to 15% and CO2 loadings from 0.2 to 0.6

The absorption reaction between aqueous NH3 and CO2 was studied using the Wetted Wall Column. A total of 27 different cases are investigated in the region defined by temperatures from 15 °C to 35 °C, NH3 concentrations from 5% to 15%, which are the typical solvent conditions in absorption columns, and lastly CO2 loadings from 0.2 to 0.6. The resulting overall mass transfer coefficient of absorption measured follows the trends described by the modelling of the reactor and the equations used to describe the rate of the absorption reactions. Moreover, the overall mass transfer coefficient of absorption is in agreement with data available in the literature, valid in smaller portions of the investigated region. From the data analysis, the kinetics of the absorption reactions in the liquid phase is characterized. The equation proposed to fit the data is a power law equation which reproduces the experimental results measured at different CO2 loadings. This represents a novelty because in literature the kinetic model of the reaction is usually fitted only to data for unloaded solutions (CO2 loading equal to zero). Hence, in this case there is an experimental evidence that the kinetic model holds true in every loading conditions. The kinetic model intercept the values found in literature in every range of concentration. Consequently, the model is valid in every conditions and the rate of the reaction between NH3 and CO2 in liquid phase is described with an Arrhenius constant with a pre-exponential factor of $1.41 \times 10^{8}$ [mol/(m$^3$s)] and an activation energy of 60,680 [J/mol], a linear dependence on the CO2 concentration and a dependence on the NH3 with an exponent $\gamma = 1.89$. The proposed equation is found to be appropriate for implementation into process simulation software.
Exploring the effects of ZVI addition on resource recovery in the anaerobic digestion process

The influence of Zero Valent Iron (ZVI) addition on the potential resource recovery during the anaerobic digestion (AD) of domestic waste sludge is assessed. Potentially recoverable resources analyzed were nutrients such as struvite to recover P, and energy as biogas to recover C. Short term (biochemical methane potential tests, BMP) and long term (AD1, AD2) experiments are conducted using two types of set-up (batch, continuous). Process data (influent, effluent and biogas) is continuously collected and the dry digested sludge is analyzed by XPS. A mathematical model is developed based on a modified version of the Anaerobic Digestion Model No 1 upgraded with an improved physicochemical description, ZVI corrosion, propionate uptake enhancement and multiple mineral precipitation. The results of all experiments show that ZVI addition increases methane production and promotes the formation of siderite (FeCO3) and vivianite (Fe3(PO4)2), which causes changes in the biogas composition (%CH4 versus %CO2) and reduces P release. The model can satisfactorily reproduce the dynamics of AD processes, nutrient release, pH and methanogenesis in AD1. The proposed approach also describes the changes in the overall performance of the process because of ZVI addition in AD2. A model-based scenario analysis is included balancing chemical-ZVI addition and increased methane production/struvite precipitation. This scenario analysis allows concluding that: (a) the improvement of methane production does not compensate the costs of ZVI purchase, and (b) ZVI dramatically decreases the P recovery potential in the digestate of the AD systems. This is the first study to experimentally and mathematically describe the effect of ZVI on biogas production/composition and on the fate of phosphorus compounds, and its potential implications for potential energy and phosphorus recovery in AD systems.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Instituto de Catálisis y Petroleoquímica, Universidad Rey Juan Carlos
Authors: Puyol, D. (Ekstern), Flores-Alsina, X. (Intern), Segura, Y. (Ekstern), Molina, R. (Ekstern), Padrino, B. (Ekstern), Fierro, J. L. G. (Ekstern), Gernaey, K. V. (Intern), Melero, J. A. (Ekstern), Martinez, F. (Ekstern)
Pages: 703-711
Publication date: 2018
Abstract We investigate the influence of controlled uniaxial extension on various flow induced phenomena in semidilute solutions of ultra high molecular weight polyethylene (UHMwPE). Concentrations range from 9 w% to 29 w% and the choice of solvent is paraffin oil (PO). The start-up extensional behavior is measured at various Hencky strain rates $\dot{\varepsilon}$ and at two different temperatures ($150 ^\circ C$ and $170 ^\circ C$) well above the melting point. At $\varepsilon > 0.9$ the qualitative behavior of the samples differ significantly depending on the imposed conditions and the concentration of the samples. Overall we propose two flow scenarios: Scenario 1 - flow induced phase separation resulting in an unstable bulky filament and Scenario 2 - flow induced phase separation and crystallization resulting in a stable deformation and a smooth strongly strain hardening filament. Scenario 2 is observed only at $150 ^\circ C$ at high $\dot{\varepsilon}$ and high concentrations. Scenario 1, observed at both temperatures, is most pronounced at low rates and/or high concentrations.
Gene stacking of multiple traits for high yield of fermentable sugars in plant biomass

Background: Second-generation biofuels produced from biomass can help to decrease dependency on fossil fuels, bringing about many economic and environmental benefits. To make biomass more suitable for biorefinery use, we need a better understanding of plant cell wall biosynthesis. Increasing the ratio of C6 to C5 sugars in the cell wall and decreasing the lignin content are two important targets in engineering of plants that are more suitable for downstream processing for second-generation biofuel production.

Results: We have studied the basic mechanisms of cell wall biosynthesis and identified genes involved in biosynthesis of pectic galactan, including the GALS1 galactan synthase and the UDP-galactose/UDP-rhamnose transporter URGT1. We have engineered plants with a more suitable biomass composition by applying these findings, in conjunction with synthetic biology and gene stacking tools. Plants were engineered to have up to fourfold more pectic galactan in stems by overexpressing GALS1, URGT1, and UGE2, a UDP-glucose epimerase. Furthermore, the increased galactan trait was engineered into plants that were already engineered to have low xylan content by restricting xylan biosynthesis to vessels where this polysaccharide is essential. Finally, the high galactan and low xylan traits were stacked with the low lignin trait obtained by expressing the QsuB gene encoding dehydroshikimate dehydratase in lignifying cells.

Conclusion: The results show that approaches to increasing C6 sugar content, decreasing xylan, and reducing lignin content can be combined in an additive manner. Thus, the engineered lines obtained by this trait-stacking approach have substantially improved properties from the perspective of biofuel production, and they do not show any obvious negative growth effects. The approach used in this study can be readily transferred to bioenergy crop plants.
Global Sensitivity Analysis as Good Modelling Practices tool for the identification of the most influential process parameters of the primary drying step during freeze-drying

Pharmaceutical batch freeze-drying is commonly used to improve the stability of biological therapeutics. The primary drying step is regulated by the dynamic settings of the adaptable process variables, shelf temperature $T_s$ and chamber pressure $P_c$. Mechanistic modelling of the primary drying step leads to the optimal dynamic combination of these adaptable process variables in function of time. According to Good Modelling Practices, a Global Sensitivity Analysis (GSA) is essential for appropriate model building. In this study, both a regression-based and variance-based GSA were conducted on a validated mechanistic primary drying model to estimate the impact of several model input parameters on two output variables, the product temperature at the sublimation front $T_i$ and the sublimation rate $V_{\text{subl}}$. $T_s$ was identified as most influential parameter on both $T_i$ and $V_{\text{subl}}$, followed by $P_c$ and the dried product mass transfer resistance $\alpha_{R_p}$ for $T_i$ and $V_{\text{subl}}$, respectively. The GSA findings were experimentally validated for $V_{\text{subl}}$ via a Design of Experiments (DoE) approach. The results indicated that GSA is a very useful tool for the evaluation of the impact of different process variables on the model outcome, leading to essential process knowledge, without the need for time-consuming experiments (e.g., DoE).

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Ghent University
Authors: Van Bockstal, P. (Ekstern), Mortier, S. T. F. (Ekstern), Corver, J. (Ekstern), Nopens, I. (Ekstern), Gernaey, K. V. (Intern), De Beer, T. (Ekstern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
A nodal high-order discontinuous Galerkin finite element (DG-FE) method is presented to solve the equilibrium-dispersive model of chromatography with arbitrary high-order accuracy in space. The method can be considered a high-order extension to the total variation diminishing (TVD) framework used by Javeed et al. (2011a,b, 2013) with an efficient quadrature-free implementation. The framework is used to simulate linear and non-linear multicomponent chromatographic systems. The results confirm arbitrary high-order accuracy and demonstrate the potential for accuracy and speed-up gains obtainable by switching from low-order methods to high-order methods. The results reproduce an analytical solution and are in excellent agreement with numerical reference solutions already published in the literature.

**General information**

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**Organisations:** Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre

**Authors:** Meyer, K. (Intern), Huusom, J. K. (Intern), Abildskov, J. (Ekstern)

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- Web of Science (2016): Indexed yes
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- Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
- Web of Science (2015): Indexed yes
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- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.176 SNIP 1.796
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.154 SNIP 2.166
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 1.293 SNIP 2.127
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.625 SNIP 1.959
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.304 SNIP 1.936
- Scopus rating (2005): SJR 1.314 SNIP 1.953
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.125 SNIP 1.908
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 1.348 SNIP 1.936
- Scopus rating (2002): SJR 1.042 SNIP 0.92
- Web of Science (2002): Indexed yes
- Scopus rating (2001): SJR 0.955 SNIP 0.728
- Web of Science (2001): Indexed yes
- Scopus rating (2000): SJR 1.366 SNIP 1.025
High-pressure pyrolysis and oxidation of ethanol
The pyrolysis and oxidation of ethanol has been investigated at temperatures of 600–900K, a pressure of 50bar and 
residence times of 4.3–6.8s in a laminar flow reactor. The experiments, conducted with mixtures highly diluted in nitrogen, 
covered fuel-air equivalence ratios (\(\Phi\)) of 0.1, 1.0, 43, and \(\infty\). Ethanol pyrolysis was observed at temperatures above 
850K. The onset temperature of ethanol oxidation occurred at 700–725K over a wide range of stoichiometries. A 
considerable yield of aldehydes was detected at intermediate temperatures. A detailed chemical kinetic model was 
developed and evaluated against the present data as well as ignition delay times and flame speed measurements from 
literature. The model predicted the onset of fuel conversion and the composition of products from the flow reactor 
experiments fairly well. It also predicted well ignition delays above 900K whereas it overpredicted reported flame speeds 
slightly. The results of sensitivity analyses revealed the importance of the reaction between ethanol and the hydroperoxyl 
radical for ignition at high pressure and intermediate temperatures. An accurate determination of the rate coefficients for 
this reaction is important to improve the reliability of modeling predictions.
Hydrate thermal dissociation behavior and dissociation enthalpies in methane-carbon dioxide swapping process

The swapping of methane with carbon dioxide in hydrate has been proposed as a potential strategy for geologic sequestration of carbon dioxide and production of methane from natural hydrate deposits. However, this strategy requires a better understanding of the thermodynamic characteristics of CH₄ and CO₂ hydrate as well as (CH₄ + CO₂) or (CH₄ + CO₂ + N₂) mixed hydrates (since (CO₂ + N₂) gas mixture is often used as the swapping gas), along with the thermal physics property changes during gas exchange. In this study, a high pressure micro-differential scanning calorimetry (HP μ-DSC) was performed on synthesized gas hydrates to investigate the dissociation behavior of various hydrates. The hydrate dissociation enthalpies were determined by both μ-DSC measurement and Clapeyron equation. For the single guest molecule hydrate system, the average dissociation enthalpies of CH₄ hydrate and CO₂ hydrate measured by integrating the endothermic peak area are 55.01 kJ·mol⁻¹ and 58.96 kJ·mol⁻¹, respectively, which are very close to the values calculated by Clapeyron equation. However, in the multicomponent guest hydrates system, the μ-DSC measured dissociation enthalpies of the (CH₄ + CO₂) binary hydrates and (CH₄ + CO₂ + N₂) ternary hydrates are a little higher than that of Clapeyron equation, it was found that their dissociation enthalpies are located between the limiting values of pure CH₄ hydrate and CO₂ hydrate, increasing with the mole fraction of CO₂ in hydrate phase. By monitoring the heat flow changes with the μ-DSC apparatus, it was observed that there was no noticeable dissociation or reformation process of hydrate occurring in the CH₄ − CO₂/(CO₂ + N₂) swapping, which indicates that most CH₄ hydrate forms (CH₄ + CO₂) or (CH₄ + CO₂ + N₂) mixed hydrates directly instead of dissociating into liquid water or ice first. The dissociation equilibrium data obtained from the endothermic thermograms of the mixed hydrates after CO₂ and (CO₂ + N₂) swapping demonstrates that about 66% and 85% of CH₄ in hydrate phase are replaced, respectively.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Mu, L. (Intern), von Solms, N. (Intern)
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Publication date: 2018

Hydrothermal Liquefaction of Enzymatic Hydrolysis Lignin: Biomass Pretreatment Severity Affects Lignin Valorization

Alkaline hydrothermal liquefaction (HTL) of lignin-rich enzymatic hydrolysis residues (EnzHR) from wheat straw and Miscanthus × giganteus was performed at 255, 300, and 345 °C to investigate valorization of this side-stream from second-generation bioethanol production. The EnzHR were from biomass hydrothermally pretreated at two different levels of severity (190 °C, 10 min; 195 °C, 15 min), and HTL at 300 °C of these EnzHR showed the most effective lignin depolymerization of the low severity EnzHR for both wheat straw and Miscanthus. The degree of depolymerization during HTL was temperature dependent and was not complete after 20 min at 255 °C, most distinctly for the Miscanthus EnzHR. The yields of 128 monomeric products quantified by gas chromatography–mass spectrometry were up to 15.4 wt % of dry matter. Principal component analysis of the quantified compounds showed that nonlignin HTL products are main contributors to the variance of the HTL products from the two biomasses. The chemically modified lignin polymer was found to have increased thermal stability after HTL. Analytical pyrolysis was applied to investigate the chemical composition of a larger fraction of the products. Analytical pyrolysis contributed with additional chemical information as well as confirming trends seen from quantified monomers. This work is relevant for future lignin valorization in biorefineries based on current second-generation bioethanol production.

Influence of Adsorption and Capillary Pressure on Phase Equilibria Inside Shale Reservoirs

Due to the small pore sizes and organic content of shale, capillary pressure and adsorption are two effects that should be taken into account in the study of phase equilibrium inside shale. The inclusion of both effects in the phase equilibrium modeling can shed light on how bulk phase composition inside the porous media changes with temperature and pressure.
and how the phase equilibrium changes accordingly. In the long run, such a model can be used in reservoir simulation for more complicated analysis. In this study, we present a calculation method that can effectively include adsorption and capillarity. We propose to introduce an excess adsorbed phase and treat the remaining substance inside the pores as a bulk phase (gas, liquid, or both) in order to make the mass balance formulation simpler. The adsorbed phase is modeled by the Multicomponent Langmuir (ML) equation for its simplicity and computational efficiency. A more theoretical adsorption model, the multicomponent potential theory of adsorption (MPTA), is used to determine the parameters of the simpler ML equation. The liquid and gas phases are described by the Peng-Robinson equation of state and the capillary pressure across their interface is taken into account. A flash algorithm by alternately updating the adsorbed phase amount and the fugacities in the bulk phases has been developed. The flash algorithm is used to analyze some representative systems (from binary, ternary to low-GOR and high-GOR model reservoir fluid systems) for the phase equilibrium inside porous media. The results show that adsorption and capillary pressure can significantly change the bulk phase composition and thus its corresponding phase envelope. Since the adsorption varies at different temperature and pressure conditions, the extent of change in the phase envelope is different. In general, a much shrunk phase envelope with a shifted critical point is observed. The heavier components are preferentially adsorbed in the whole pressure and temperature range studied here. At high pressure and low temperature, the selectivity towards heavier components is moderate in comparison to the that at low pressure and high temperature. The adsorption effects are stronger for the gas bulk phase region, leading to bigger changes in the gas phase composition and the shift of the dew point curve. PVT simulations of two model reservoir fluid systems show significant change in the results when capillary pressure and adsorption are included.

General information
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Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering
Authors: Sandoval, D. R. (Intern), Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
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Web of Science (2016): Indexed yes
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Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.05
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
**Influence of H2O and H2S on the Composition, Activity, and Stability of Sulfided Mo, CoMo, and NiMo Supported on MgAl2O4 for Hydrodeoxygenation of Ethylene Glycol**

In this work, density functional theory (DFT), catalytic activity tests, and in-situ X-ray absorption spectroscopy (XAS) was performed to gain detailed insights into the activity and stability of MoS2, Ni-MoS2, and Co-MoS2 catalysts used for hydrodeoxygenation (HDO) of ethylene glycol upon variation of the partial pressures of H2O and H2S. The results show high water tolerance of the catalysts and highlight the importance of promotion and H2S level during HDO.

DFT calculations unraveled that the active edge of MoS2 could be stabilized against S-O exchanges by increasing the partial pressure of H2S or by promotion with either Ni or Co. The Mo, NiMo, and CoMo catalysts of the present study were all active and fairly selective for ethylene glycol HDO at 400 °C, 27 bar H2, and 550-2200 ppm H2S, and conversions of ≈ 50-100%. The unpromoted Mo/MgAl2O4 catalyst had a lower stability and activity per gram catalyst than the promoted analogues. The NiMo and CoMo catalysts produced ethane, ethylene, and C1 cracking products with a C2/C1 ratio of 1.5-2.0 at 550 ppm H2S. This ratio of HDO to cracking could be increased to ≈ 2 at 2200 ppm H2S which also stabilized the activity. Removing H2S from the feed caused severe catalyst deactivation. Both DFT and catalytic activity tests indicated that increasing the H2S concentration increased the concentration of SH groups on the catalyst, which correspondingly activated and stabilized the catalytic HDO performance. In-situ XAS further supported that the catalysts were tolerant towards water when exposed to increasing water concentration with H2O/H2S ratios up to 300 at 400-450 °C.

Raman spectroscopy and XAS showed that MoS2 was present in the prepared catalysts as small and highly dispersed particles, probably owing to a strong interaction with the support. Linear combination fitting (LCF) analysis of the X-ray absorption near edge structure (XANES) spectra obtained during in-situ sulfidation showed that Ni was sulfided faster than Mo and CoMo, and that Mo was sulfided faster when promoted with Ni. Extended X-ray absorption fine structure (EXAFS) results showed the presence of MoS2 in all sulfided catalysts. Sulfided CoMo was present as a mixture of CoMoS and Co9S8, whereas sulfided NiMo was present as NiMoS.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Center for Electron Nanoscopy, Karlsruhe Institute of Technology KIT, SLAC National Accelerator Laboratory, Haldor Topsoe AS
Authors: Dabros, T. M. H. (Intern), Gaur, A. (Ekstern), Pintos, D. G. (Ekstern), Sprenger, P. (Ekstern), Høj, M. (Intern), Hansen, T. W. (Intern), Studt, F. (Ekstern), Gabrielsen, J. (Ekstern), Grunwaldt, J. (Ekstern), Jensen, A. D. (Intern)
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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
Influence of Preoxidation on High-Temperature Corrosion of a FeCrAl Alloy Under Conditions Relevant to Biomass Firing

Preoxidation of a commercial FeCrAl alloy (Kanthal APM) was evaluated as a surface modification approach to reduce alkali chloride-induced corrosion during biomass firing in power plants. Samples of the alloy preoxidized at 900 °C in O₂ or O₂ + 10 vol% H₂O₂ and at 1100 °C in O₂, were coated with KCl and exposed at 560 °C to a gas mixture comprising of 12 vol% CO₂, 6 vol% O₂, 3 vol% H₂O, 400 ppmv HCl and 60 ppmv SO₂. The oxide formed at 1100 °C showed no reactivity with the corrosive species. By contrast, all samples preoxidized at 900 °C suffered severe attack, resulting in formation of Fe-, Cr- and Al-containing corrosion products in a heterogeneous morphology, similar to non-preoxidized samples. The observed differences with respect to the degree of corrosion attack on the preoxidized samples are discussed in terms of the composition and thickness of the different types of Al₂O₃ layers obtained by the preoxidation treatment.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Department of Mechanical Engineering, Materials and Surface Engineering, CHEC Research Centre
Authors: Okoro, S. C. (Intern), Montgomery, M. (Intern), Jappe Frandsen, F. (Intern), Pantleon, K. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.22 SJR 0.659 SNIP 0.865
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.829 SNIP 1.177 CiteScore 1.38
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.826 SNIP 1.345 CiteScore 1.49
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.897 SNIP 1.715 CiteScore 1.67
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.961 SNIP 1.901 CiteScore 1.43
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.818 SNIP 1.746 CiteScore 1.69
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.682 SNIP 1.233
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.754 SNIP 1.635
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.371 SNIP 2.163
Scopus rating (2007): SJR 0.93 SNIP 1.544
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.815 SNIP 1.708
Scopus rating (2005): SJR 1.492 SNIP 1.927
Investigation of curing rates of bio-based thiol-ene films from diallyl 2,5-furandicaboxylate

The bio-based monomer, 2,5-furandicarboxylic acid, has been adapted to classic thiol-ene chemistry by derivatization of the acid with allyl alcohol. This new monomer has allowed for the synthesis of new thermoset systems, capable of forming green, sustainable materials through UV-crosslinking. In this study, the synthesis of the new monomer along with thorough kinetic studies of the new thermoset systems are presented. In order to determine kinetic values for the systems, all reactions have been followed by real-time FT-IR. Initially, a study of three different photoinitiators is performed on a classic TEMPICTATATO system, in order to determine the superior initiator for the new systems. The new monomer is crosslinked with five different thiol compounds in both stoichiometric and off-stoichiometric ratios, yielding an array of bio-based thermosets. The properties of these systems are determined through DSC, TGA and tensile testing, allowing determination of the systems with superior properties. In general, most systems proved to cure fully, with the exception of issues encountered from thiols with long ethoxylated chains.
Lignin from hydrothermally pretreated grass biomass retards enzymatic cellulose degradation by acting as a physical barrier rather than by inducing nonproductive adsorption of enzymes

Lignin is known to hinder efficient enzymatic conversion of lignocellulose in biorefining processes. In particular, nonproductive adsorption of cellulases onto lignin is considered a key mechanism to explain how lignin retards enzymatic cellulose conversion in extended reactions. Lignin-rich residues (LRRs) were prepared via extensive enzymatic cellulose degradation of corn stover (Zea mays subsp. mays L.), Miscanthus × giganteus stalks (MS) and wheat straw (Triticum aestivum L.) (WS) samples that each had been hydrothermally pretreated at three severity factors (log \( R_0 \)) of 3.65, 3.83 and 3.97. The LRRs had different residual carbohydrate levels—the highest in MS; the lowest in WS. The residual carbohydrate was not traceable at the surface of the LRRs particles by ATR-FTIR analysis. The chemical properties of the lignin in the LRRs varied across the three types of biomass, but monolignols composition was not affected by the severity factor. When pure cellulose was added to a mixture of LRRs and a commercial cellulolytic enzyme preparation, the rate and extent of glucose release were unaffected by the presence of LRRs regardless of biomass type and severity factor, despite adsorption of the enzymes to the LRRs. Since the surface of the LRRs particles were covered by lignin, the data suggest that the retardation of enzymatic cellulose degradation during extended reaction on lignocellulosic substrates is due to physical blockage of the access of enzymes to the cellulose caused by the gradual accumulation of lignin at the surface of the biomass particles rather than by nonproductive enzyme adsorption. The study suggests that lignin from hydrothermally pretreated grass biomass retards enzymatic cellulose degradation by acting as a physical barrier blocking the access of enzymes to cellulose rather than by inducing retardation through nonproductive adsorption of enzymes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Aarhus University, University of Copenhagen, Technical University of Denmark
Number of pages: 13
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Main Research Area: Technical/natural sciences
Liquid-to-solid ratio control as an advanced process control solution for continuous twin-screw wet granulation

Assuring compliance of intermediate and final quality attributes in a continuous pharmaceutical manufacturing campaign is of utmost importance. Application of corrective actions might be required in real-time. This work exemplifies the steps needed to identify a linear pulse transfer function for the dynamic behavior of the granule liquid-to-solid ratio (w) at the end of the granulation unit of a commercial ConsiGma™-25 production line. Near-infrared spectroscopy was used to monitor...
the granule composition in-line. The outcome for both the tracking and regulator problem using either conventional or model predictive control was implemented and evaluated. Dynamic setpoints were correctly followed and an RMSE of 0.25\(w\) with respect to the setpoint was obtained when inducing artificial disturbances. Important practical challenges were also tackled. Examples are fouling, computational limitations, and the limited flexibility of the automation software. Applying the proposed advanced process control solution offers an answer to upstream material flow rate deviations.

**General information**

State: Accepted/In press  
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Ghent University  
Authors: Nicolaï, N. (Ekstern), Leersnyder, F. D. (Ekstern), Copot, D. (Ekstern), Stock, M. (Ekstern), Ionescu, C. M. (Ekstern), Gernaey, K. V. (Intern), Nopens, I. (Ekstern), Beer, T. D. (Ekstern)  
Number of pages: 15  
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**Publication information**

Journal: AIChE Journal  
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BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
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Web of Science (2017): Indexed Yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 1.004 SNIP 1.234 CiteScore 2.31  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 1.083 SNIP 1.423  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 1.192 SNIP 1.437  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 1.287 SNIP 1.428  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.256 SNIP 1.341  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.483 SNIP 1.612
Low energy recycling of ionic liquids via freeze crystallization during cellulose spinning

A new method for recycling ionic liquids (ILs) from a cellulose spinning process is suggested. The method involves the combination of freeze crystallization and evaporation of H₂O from IL + H₂O mixtures to recycle the ILs. Processes with EmimAc and EmimDep were used as references to develop this IL recycling method. EmimAc + 12.5 wt% H₂O and EmimDep + 4 wt% H₂O were selected for a quantitative mass and energy analysis of the cellulose spinning and IL recycling process (the maximal initial H₂O levels in the ILs + H₂O mixtures for cellulose dissolution were determined experimentally). The energy requirement for the freeze crystallization + evaporation method was compared to evaporation only for recycling of EmimAc and EmimDep. To produce 1 kg dry cellulose fiber, 45.4 MJ and 62.6 MJ are required for recycling EmimAc and EmimDep respectively by the freeze crystallization + evaporation recycling method. Using evaporation only, 66.9 MJ is required for EmimAc recycling and 99.9 MJ for EmimDep recycling per kg cellulose fiber produced. Thus, to fabricate 1 kg dry cellulose fiber using freeze crystallization + evaporation rather than evaporation, 21.5 MJ can be saved for EmimAc and 37.3 MJ for EmimDep recycling. We also show that compared to a classical Lyocell fiber production method using N-methylmorpholine-N-oxide (NMMO) as solvent, use of ILs is energy saving in itself. Hence, significantly less H₂O is required in the cellulose spinning process with ILs than with NMMO, and in turn less H₂O has to be evaporated for the solvent recycling.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, CERE – Center for Energy Ressources Engineering, Chinese Academy of Sciences
Authors: Liu, Y. (Intern), Meyer, A. S. (Intern), Nie, Y. (Ekstern), Zhang, S. (Ekstern), Thomsen, K. (Intern)
Pages: 493-501
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Green Chemistry
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ISSN (Print): 1463-9262
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.564 SNIP 2.019
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.477 SNIP 1.901 CiteScore 8.21
Measurements of the NOx precursors and major species concentrations above the grate at a waste-to-energy plant

Satisfactory results from modelling of NOx formation in CFD during combustion of Municipal Solid Waste (MSW) in grate-fired waste-to-energy plants is highly depended on accurate descriptions of the temperature field in the free-board above the waste bed. Accurate modelling of the temperature field relies on an accurate determination of the boundary conditions; the species concentration, gas temperature and gas velocity from the waste bed into the computational domain. In this study the gas temperature and the gas concentration profiles of O2, H2O, CO, CO2, CH4, C2H2, C2H4, NH3 and HCN along the waste bed were measured. The measurements were performed on a 9 ton/h grate-fired waste-to-energy plant, Affald+ unit 4 in Denmark. The species concentration profiles were determined by gas extraction using a 6 m water cooled probe and FTIR spectroscopy, while the gas temperatures were determined by suction pyrometer. The major combustible gasses were determined to be CO, CH4 and C2H4, which are only found above the first half of the grate. Furthermore, it was determined that during grate-fired MSW combustion the majority of the NOx precursors are released as NH3; more than 80%. The influence of NOx precursor composition on the NOx formation was examined through CHEMKIN simulations. It was shown that for reliable modelling of the NO formation at high excess air ratios, λ > 1.1, it is important to determine the correct ratio between NH3 and HCN. The importance of an accurate precursor determination increases considerably with decreasing temperatures.
Mechanistic modeling of cyclic voltammetry: A helpful tool for understanding biosensor principles and supporting design optimization

Abstract Design, optimization and integration of biosensors hold a great potential for the development of cost-effective screening and point-of-care technologies. However, significant progress in this field can still be obtained on condition that sufficiently accurate mathematical models will be developed. Herein, we present a novel approach for the improvement of mechanistic models which do not only combine the fundamental principles but readily incorporate the results of electrochemical and morphological studies. The first generation glucose biosensors were chosen as a case study for model development and to perform cyclic voltammetry (CV) measurements. As initial step in the model development we proposed the interpretation of experimental voltammograms obtained in the absence of substrate (glucose). The model equations describe dynamic diffusion and reaction of the involved species (oxygen, oxidized/reduced forms of the mediator - Prussian Blue/Prussian White). Furthermore, the developed model was applied under various operating conditions as a crucial tool for biosensor design optimization. The obtained qualitative and quantitative dependencies towards amperometric biosensors design optimization were independently supported by results of cyclic voltammetry and multi-analytical studies, such as scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS). Remarkably, a linear response of the optimized biosensors tested at the applied voltage (~0.14V) in the presence of the glucose was obtained from 10^{-3} to 10^{-5}M (relative standard deviation (RSD) <7% per electrode). We believe that the presented model can be used to determine the exact mechanism driving the electrochemical reactions and to identify critical system parameters affecting the biosensor response that would significantly contribute to the knowledge on biosensing, device design and bioengineering strategies in the future.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Leibniz-Institute for New Materials (INM), Saarbrucken, Università degli Studi di Roma Tor Vergata
Authors: Semenova, D. (Intern), Zubov, A. (Intern), Silina, Y. E. (Ekstern), Micheli, L. (Ekstern), Koch, M. (Ekstern), Fernandes, A. C. (Intern), Gernaey, K. V. (Intern)
Pages: 945–955
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Sensors and Actuators B: Chemical
Volume: 259
ISSN (Print): 0925-4005
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.07 SJR 1.333 SNIP 1.463
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.25 SNIP 1.509 CiteScore 4.84
Melting behaviour of raw materials and recycled stone wool waste

Stone wool is a widely used material for building insulation, to provide thermal comfort along with fire stability and acoustic comfort for all types of buildings. Stone wool waste generated either during production or during renovation or demolition of buildings can be recycled back into the stone wool melt production. This study investigates and compares the thermal response and melting behaviour of a conventional stone wool charge and stone wool waste. The study combines differential scanning calorimetry (DSC), hot stage microscopy (HSM) and X-ray diffraction (XRD). DSC reveals that the conventional charge and stone wool waste have fundamentally different thermal responses, where the charge experiences gas release, phase transition and melting of the individual raw materials. The stone wool waste experiences glass transition, crystallization and finally melting. Both DSC and HSM measurements indicates that the wool waste
initiates melting at a lower temperature than the conventional charge. Also DSC measurements show that the wool waste requires less energy for heating and melting than the conventional charge, making stone wool waste recycling desirable both for environmental and for process purposes.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Energy Conversion and Storage, Mixed Conductors, Rockwool International
Authors: Schultz-Falk, V. (Intern), Agersted, K. (Ekstern), Jensen, P. A. (Intern), Solvang, M. (Ekstern)
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**Publication information**

Journal: Journal of Non-Crystalline Solids
Volume: 485
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.02 SJR 0.692 SNIP 1.163
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.684 SNIP 1.083 CiteScore 1.85
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.803 SNIP 1.194 CiteScore 1.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.822 SNIP 1.19 CiteScore 1.79
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.758 SNIP 1.124 CiteScore 1.64
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.836 SNIP 1.272 CiteScore 1.7
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.911 SNIP 1.128
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.924 SNIP 0.993
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.957 SNIP 1.2
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.95 SNIP 1.082
Scopus rating (2006): SJR 0.887 SNIP 1.158
Scopus rating (2005): SJR 0.986 SNIP 1.149
Scopus rating (2004): SJR 0.992 SNIP 1.216
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.362 SNIP 1.308
Scopus rating (2002): SJR 0.861 SNIP 1.051
Scopus rating (2001): SJR 1.099 SNIP 1.09
Scopus rating (2000): SJR 0.948 SNIP 1.074
Membrane separation of enzyme-converted biomass compounds: Recovery of xylose and production of gluconic acid as a value-added product.

The purpose of the present study was to assess the efficiency of enzyme-assisted nanofiltration for separation of xylose from glucose present in genuine biorefinery liquors obtained from hydrothermal pretreatment of wheat straw, corn stover and Miscanthus stalks. Glucose oxidase and catalase were used to convert the glucose contained in the liquors into gluconic acid, so xylose could be more easily recovered in the subsequent nanofiltration. Subjecting the biomass liquors to dilute acid treatment and centrifugation before the enzymatic reaction and filtration led to maximum biocatalytic performance of the membrane bioreactor (negligible fouling and no enzyme activity loss) during five consecutive reaction-filtration cycles. The best separation factor of gluconic acid over xylose in the subsequent nanofiltration was 2.7, 2.5 and 2.2 for wheat straw, corn stover and Miscanthus stalks, respectively. All represented a significant improvement compared to the benchmark separation of xylose and glucose, in which case the separation factor was only 1.4. However, the higher ionic strength of the biomass liquors compared to the pure model solution probably led to a less negative zeta potential of the nanofiltration membrane, which significantly reduced the xylose purification performance as compared to the model system, for which the separation factor was 34.
Methodology for Developing a Diesel Exhaust After Treatment Simulation Tool

A methodology for the development of catalyst models is presented. Also, a methodology of the implementation of such models into a modular simulation tool, which simulates the units in succession, is presented. A case study is presented illustrating how suitable models can be found and used for simulations. Such simulations illustrate the behavior of the individual units and the overall system. It is shown how, by simulating the units in succession, the entire after treatment system can be tested and optimized, because the integration makes it possible to observe the effect of the modules on one another.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Technical University of Denmark
Authors: Christiansen, T. (Ekstern), Jensen, J. (Ekstern), Åberg, A. (Intern), Abildskov, J. (Ekstern), Huusom, J. (Intern)
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Journal: SAE International Journal of Commercial Vehicles
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Original language: English
Modelling, Simulation tool, Diesel exhaust after treatment
DOIs:
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Source: RIS
Source-ID: urn:E6A6C7CF1462437DB4FAAA4C7956D4FC
Publication: Research - peer-review › Journal article – Annual report year: 2018
Modeling Electron Competition among Nitrogen Oxides Reduction and N\textsubscript{2}O Accumulation in Hydrogenotrophic Denitrification

Hydrogenotrophic denitrification is a novel and sustainable process for nitrogen removal, which utilizes hydrogen as electron donor and carbon dioxide as carbon source. Recent studies have shown that nitrous oxide (N\textsubscript{2}O), a highly undesirable intermediate and potent greenhouse gas, can accumulate during this process. In this work, a new mathematical model is developed to describe nitrogen oxides dynamics, especially N\textsubscript{2}O, during hydrogenotrophic denitrification for the first time. The model describes electron competition among the four steps of hydrogenotrophic denitrification through decoupling hydrogen oxidation and nitrogen reduction processes using electron carriers, in contrast to the existing models that couple these two processes and also do not consider N\textsubscript{2}O accumulation. The developed model satisfactorily describes experimental data on nitrogen oxides dynamics obtained from two independent hydrogenotrophic denitrifying cultures under various hydrogen and nitrogen oxides supplying conditions, suggesting the validity and applicability of the model. The results indicated that N\textsubscript{2}O accumulation would not be intensified under hydrogen limiting conditions, due to the higher electron competition capacity of N\textsubscript{2}O reduction in comparison to nitrate and nitrite reduction during hydrogenotrophic denitrification. The model is expected to enhance our understanding of the process during hydrogenotrophic denitrification and the ability to predict N\textsubscript{2}O accumulation.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, University of Technology, Sydney, University of Antwerp, Hunan University, Sichuan University, Tongji University
Pages: 978–988
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Main Research Area: Technical/natural sciences

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Journal: Biotechnology and Bioengineering
Volume: 115
Issue number: 4
ISSN (Print): 1097-0290
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.411 SNIP 1.163
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.613 SNIP 1.37 CiteScore 4.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.589 SNIP 1.401 CiteScore 4.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.621 SNIP 1.425 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.639 SNIP 1.366 CiteScore 4.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.668 SNIP 1.483 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Modeling nitrogen chemistry in combustion

Understanding of the chemical processes that govern formation and destruction of nitrogen oxides (NOx) in combustion processes continues to be a challenge. Even though this area has been the subject of extensive research over the last four decades, there are still unresolved issues that may limit the accuracy of engineering calculations and thereby the potential of primary measures for NOx control. In this review our current understanding of the mechanisms that are responsible for combustion-generated nitrogen-containing air pollutants is discussed. The thermochemistry of the relevant nitrogen compounds is updated, using the Active Thermochemical Tables (ATcT) approach. Rate parameters for the key gas-phase reactions of the nitrogen species are surveyed, based on available information from experiments and high-level theory. The mechanisms for thermal and prompt-NO, for fuel-NO, and NO formation via NNH or N2O are discussed, along with the chemistry of NO removal processes such as reburning and Selective Non-Catalytic Reduction of NO. Each subset of the mechanism is evaluated against experimental data and the accuracy of modeling predictions is discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Argonne National Laboratory
Authors: Glarborg, P. (Intern), Miller, J. A. (Ekstern), Ruscic, B. (Ekstern), Klippenstein, S. J. (Ekstern)
Pages: 31-68
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Progress in Energy and Combustion Science
Volume: 67
ISSN (Print): 0360-1285
Ratings:
Modeling of Pharmaceutical Biotransformation by Enriched Nitrifying Culture under Different Metabolic Conditions

Pharmaceutical removal could be significantly enhanced through cometabolism during nitrification processes. To date, pharmaceutical biotransformation models have not considered the formation of transformation products associated with the metabolic type of microorganisms. Here we report a comprehensive model to describe and evaluate the biodegradation of pharmaceuticals and the formation of their biotransformation products by enriched nitrifying cultures.
The biotransformation of parent compounds was linked to the microbial processes via cometabolism induced by ammonium-oxidizing bacteria (AOB) growth, metabolism by AOB, cometabolism by heterotrophs (HET) growth, and metabolism by HET in the model framework. The model was calibrated and validated using experimental data from pharmaceutical biodegradation experiments at realistic levels, taking two pharmaceuticals as examples, i.e., atenolol and acyclovir. Results demonstrated the good predictive performance of the established biotransformation model under different metabolic conditions, as well as the reliability of the established model in predicting different pharmaceutical biotransformations. The linear positive correlation between ammonia oxidation rate and pharmaceutical degradation rate confirmed the major role of cometabolism induced by AOB in the pharmaceutical removal. Dissolved oxygen was also revealed to be capable of regulating the pharmaceutical biotransformation cometabolically, and the substrate competition between ammonium and pharmaceuticals existed especially at high ammonium concentrations.
Modelling continuous pharmaceutical and bio-based processes at plant-wide level: A roadmap towards efficient decision-making

The importance of developing simulation models for decision making in pharmaceutical and bio-based production processes is elaborated in this article. The advantages of modelling continuous processes are outlined and certain barriers in this regard are identified. Although there have been some advancements in the field, there needs to be a larger international collaboration in this regard for providing reliable data for model validation, for development of generic model-based frameworks and implementing them in computer-aided platforms in the form of software tools.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Loughborough University
Authors: Ramin, P. (Intern), Mansouri, S. S. (Intern), Udugama, I. A. (Intern), Benyahia, B. (Ekstern), Gernaey, K. V. (Intern)
Pages: 26-30
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry Today
Volume: 36
Issue number: 2
Original language: English

Morphological, mechanical and antioxidant properties of Portuguese almond cultivars
The aim of this study was to evaluate morphological (of fruit and kernel), mechanical (namely shell rupture force) and antioxidant properties (including phenolics and flavonoid content) of five Portuguese almond cultivars, comparing them with two commercial cultivars (Glorieta and Ferragnès). Of the analyzed traits, nut and kernel dimensions varied substantially and were used to describe cultivars. However, some traditional cultivars recorded similar (Pegarinhos), or even higher (Amendoão, Casanova and Refêgo) nut and kernel weight than commercial cultivars. Furthermore, shelling percentage of traditional cultivar (Bonita) was higher than commercial cultivars. Rupture force necessary to break fruits of all traditional cultivars was higher than commercial ones, and was correlated to nut weight cultivars. The phenolics, flavonoids content and antioxidants were higher for Casanova. Parameters like high kernel weight, low percentages of
double kernels or losses during shelling and considerable higher phenolics and flavonoids content may be considered by industry during selection of almond.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Universidade de Tras-os-Montes e Alto Douro
Authors: Oliveira, I. (Ekstern), Meyer, A. S. (Intern), Afonso, S. (Ekstern), Ribeiro, C. (Ekstern), Gonçalves, B. (Ekstern)
Publication date: 2018
Main Research Area: Technical/natural sciences

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Journal: Journal of Food Science and Technology
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.43 SJR 0.544 SNIP 0.916
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.433 SNIP 0.914 CiteScore 1.08
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.506 SNIP 1.385 CiteScore 1.34
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.488 SNIP 1.01 CiteScore 1.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.395 SNIP 0.902 CiteScore 0.71
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.344 SNIP 0.668 CiteScore 0.51
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.31 SNIP 0.532
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.269 SNIP 0.454
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.205 SNIP 0.379
Scopus rating (2007): SJR 0.189 SNIP 0.398
Scopus rating (2006): SJR 0.189 SNIP 0.34
Scopus rating (2005): SJR 0.23 SNIP 0.372
Scopus rating (2004): SJR 0.224 SNIP 0.487
Scopus rating (2003): SJR 0.26 SNIP 0.695
Scopus rating (2002): SJR 0.267 SNIP 0.6
Scopus rating (2001): SJR 0.294 SNIP 0.444
Scopus rating (2000): SJR 0.212 SNIP 0.747
Scopus rating (1999): SJR 0.252 SNIP 0.621
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Almond, Antioxidant activity, Mechanical traits, Morphological characterization, Prunus dulcis, Traditional cultivars
DOIs:
Multi-function microfluidic platform for sensor integration

The limited availability of metabolite-specific sensors for continuous sampling and monitoring is one of the main bottlenecks contributing to failures in bioprocess development. Furthermore, only a limited number of approaches exist to connect currently available measurement systems with high throughput reactor units. This is especially relevant in the biocatalyst screening and characterization stage of process development. In this work, a strategy for sensor integration in microfluidic platforms is demonstrated, to address the need for rapid, cost-effective and high-throughput screening in bioprocesses. This platform is compatible with different sensor formats by enabling their replacement and was built in order to be highly flexible and thus suitable for a wide range of applications. Moreover, this re-usable platform can easily be connected to analytical equipment, such as HPLC, laboratory scale reactors or other microfluidic chips through the use of standardized fittings. In addition, the developed platform includes a two-sensor system interspersed with a mixing channel, which allows the detection of samples that might be outside the first sensor's range of detection, through dilution of the sample solution up to 10 times. In order to highlight the features of the proposed platform, inline monitoring of glucose levels is presented and discussed. Glucose was chosen due to its importance in biotechnology as a relevant substrate. The platform demonstrated continuous measurement of substrate solutions for up to 12h. Furthermore, the influence of the fluid velocity on substrate diffusion was observed, indicating the need for in-flow calibration to achieve a good quantitative output.
Multiscale Modeling of Poly(lactic acid) Production: From Reaction Conditions to Rheology of Polymer Melt

Abstract Poly(lactic acid) (PLLA) is a fully biodegradable bioplastic with promising market potential. The paper deals with systematic development and analysis of the modeling framework allowing direct mapping between PLLA production process conditions and rheological properties of the polymer melt. To achieve this, the framework builds upon three distinct elements that approach the production process from different scales: (i) macroscopic deterministic model of \(L,L\)-lactide ring opening polymerization taken from the literature, (ii) microscopic stochastic simulation of the polymerization process based on hybrid Monte Carlo approach, and (iii) mesoscopic public domain model of polymer chain reptation dynamics. Based on the input reaction conditions, the macro-scale model predicts \(L,L\)-lactide conversion and averaged molar mass of PLLA, while the micro-scale and meso-scale simulations allow prediction of full molar mass distribution and melt viscosity of the product. The developed predictive tool is validated by literature data, i.e. experimentally measured rheological characteristics of three commercial PLLA samples with different molecular architecture. Moreover, comprehensive global sensitivity analysis has been carried out to support exploration of the process conditions space in relation to target polymer melt properties. Computational efficiency of the developed model achieved so far foreshadows its potential use as soft sensor for molar mass distribution and melt viscosity in the optimization and control of PLLA production.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre
Authors: Zubov, A. (Intern), Sin, G. (Intern)
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Journal: Chemical Engineering Journal
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.16
Mussel-inspired co-deposition to enhance bisphenol A removal in a bifacial enzymatic membrane reactor

Abstract In this study, the biocatalytic membranes were prepared by ‘reverse filtration’ of laccase and subsequently various mussel-inspired coating strategies: single dopamine (DA) deposition, DA/polyethyleneimine (PEI) co-deposition, and DA/Cu2+ co-deposition, where nanofiltration (NF) membranes were used as the matrix to further exploit the potential of the biocatalytic membranes. Such prepared biocatalytic membranes were enzymatically active on both sides, making it possible to construct a bifacial enzymatic membrane reactor (EMR) for highly efficient micro-pollutants removal (taking bisphenol A (BPA) as an example). Compared with the single polydopamine (PDA) coated membrane, the biocatalytic membranes prepared by DA/PEI and DA/Cu2+ co-depositions exhibited much better performances in terms of enzyme loading, activity and permeability as well as the stability of immobilized enzyme. The BPA removal efficiency was highest for the EMR with the PDA/Cu2+ coated membrane attributed to copper-enhanced electron transfer, while it was lowest for the EMR with the PDA/PEI coated membrane due to the high diffusional resistance of the dense PDA/PEI layer. Meanwhile, the mechanism for performance deterioration of biocatalytic membrane during BPA treatment was revealed, and it was found that the trade-off between BPA removal efficiency and long-term stability could be broken by applying the bifacial EMR with PDA/Cu2+ coated membrane in flow-through mode, since the pressure-induced convective mass transfer improved the substrate accessibility to enzyme together with products removal.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre, Chinese Academy of Sciences
Near-wellbore modeling of a horizontal well with Computational Fluid Dynamics

The oil production by horizontal wells is a complex phenomenon that involves flow through the porous reservoir, completion interface and the well itself. Conventional reservoir simulators can hardly resolve the flow through the completion into the wellbore. On the contrary, Computational Fluid Dynamics (CFD) is capable of modeling the complex
interaction between the creeping reservoir flow and turbulent well flow for single phases, while capturing both the completion geometry and formation damage. A series of single phase steady-state simulations are undertaken, using such fully coupled three dimensional numerical models, to predict the inflow to the well. The present study considers the applicability of CFD for near-wellbore modeling through benchmark cases with available analytical solutions. Moreover, single phase steady-state numerical investigations are performed on a specific perforated horizontal well producing from the Siri field, offshore Denmark. The performance of the well is investigated with an emphasis on the inflow profile and the productivity index for different formation damage scenarios. A considerable redistribution of the inflow profile were found when the filtrate invasion extended beyond the tip of the perforations.

General information
State: Published
Organisations: Department of Mechanical Engineering, Scientific Computing, Fluid Mechanics, Coastal and Maritime Engineering, Department of Chemistry, CERE – Center for Energy Ressources Engineering, Technical University of Denmark, Lloyd’s Register Consulting
Authors: Szanyi, M. L. (Ekstern), Hemmingsen, C. S. (Intern), Yan, W. (Intern), Walther, J. H. (Intern), Glimberg, S. L. (Ekstern)
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Journal: Journal of Petroleum Science and Engineering
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.648 SNIP 1.41 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.746 SNIP 1.724
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.072 SNIP 1.852
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.841 SNIP 1.435
Scopus rating (2007): SJR 0.732 SNIP 1.386
New association schemes for mono-ethylene glycol: Cubic-Plus-Association parameterization and uncertainty analysis

Accurate thermodynamic predictions for systems containing glycols are essential for the design and commissioning of novel subsea natural gas dehydration units. Previously it has been shown that the Cubic-Plus-Association (CPA) equation of state can be used to model VLE, SLE and LLE for mixtures of interest to this application. Recent developments for association schemes have shown that the use of a binary association site provided improved modelling of 1-alkanols. In this work, we implement the binary association site for mono-ethylene glycol (MEG) by proposing three new association schemes (3C, 4E & 4F). New parameter sets have been regressed and uncertainty analysis, using the bootstrap methodology, was performed to obtain 95% confidence intervals for each parameter. An improved parameter set for the literature 4C scheme was also determined.

The four association schemes were tested against eight data types, with single parameter sensitivity analysis showing that new parameter sets are near optimal. The 3C scheme provides the best results for pure component properties and the liquid phase of MEG-H2O, while new 4C parameters provide the best results for the MEG-H2O (vapour phase) and MEG-nC7 LLE. For the limited ternary (MEG-H2O-CH4) data and MEG-nC6 LLE, the best results are achieved using the 4F scheme. Ternary modelling performance was further improved by using binary interaction parameters fitted to binary vapour phase data.

While each of the new parameter sets provided an improvement over the literature parameters, it was found that no specific scheme was universally the best option. Given the uncertainty ranges and inconsistency between literature data, additional experimental data are required.

Despite the lack of sufficient data, the value of the bootstrap method has been highlighted, both for finding improved parameter sets and transferring uncertainty from experimental data through to thermodynamic and process models.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources, KT Consortium
Authors: Kruger, F. (Intern), Kontogeorgis, G. M. (Intern), von Solms, N. (Intern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Online Measurement of Oxygen-Dependent Enzyme Reaction Kinetics

As the application of biocatalysis to complement conventional chemical and catalytic approaches continues to expand, an increasing number of reactions involve poorly-water soluble substrates. At required industrial concentrations necessary for
industrial implementation, this frequently leads to heterogeneous reaction mixtures composed of multiple phases. Such systems are challenging to sample and therefore it is problematic to measure representative component concentrations. In this work we demonstrate and validate an online method for following the progress of oxygen-dependent reactions through accurate measurement of the oxygen mass balance in the gas-phase of a reactor. The method was successfully validated and demonstrated using two model reactions: firstly the oxidation of glucose by glucose oxidase and secondly the Baeyer-Villiger oxidation of macrocyclic ketones to lactones. Initial reaction rate constants and time-course progressions calculated from the oxygen mass balance were validated against conventional online methods of dissolved oxygen tension and pH titration measurements. A feasible operating window as well as the sensitivity to dynamic changes of reaction rates was established by controlling oxygen transfer via the operating parameters of the reactor. Such kinetic data forms the basis for reaction characterisation, from which bottlenecks may be made evident and directed improvement strategies can be identified and implemented.

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
Authors: Meissner, M. P. (Intern), Nordblad, M. (Intern), Woodley, J. M. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.242 SNIP 0.733
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.255 SNIP 0.748 CiteScore 2.77
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.386 SNIP 0.852 CiteScore 2.88
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.622 SNIP 0.849 CiteScore 3.15
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.853 SNIP 0.902 CiteScore 3.49
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.903 SNIP 0.952 CiteScore 3.59
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.951 SNIP 0.931
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.899 SNIP 0.921
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.957 SNIP 0.869
Web of Science (2008): Indexed yes
On the origin of brittle fracture of entangled polymer solutions and melts

A novel criterion for brittle fracture of entangled polymer liquids is presented: Crack initiation follows from rupture of primary C-C bonds, when the strain energy of an entanglement segment reaches the energy of the covalent bond. Thermal fluctuations lead to a short-time concentration of the strain energy on one C-C bond of the entanglement segment, and the chain ruptures. This limits the maximum achievable stretch of entanglement segments to a critical stretch of \( f(c) \)

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Berlin Institute of Technology
Authors: Wagner, M. H. (Ekstern), Narimissa, E. (Ekstern), Huang, Q. (Intern)
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Journal: Journal of Rheology
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 1.414 SNIP 1.553
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.413 SNIP 1.573 CiteScore 2.67
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.692 SNIP 1.584 CiteScore 3.29
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.297 SNIP 1.583 CiteScore 2.96
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.347 SNIP 1.62 CiteScore 2.72
Optical investigation of gas-phase KCl/KOH sulfation in post flame conditions

A counter-flow reactor setup was designed to investigate the gas-phase sulfation and homogeneous nucleation of potassium salts. Gaseous KOH and KCl were introduced into the post-flame zone of a laminar flat flame. The hot flame products mixed in the counter-flow with cold N₂, with or without addition of SO₂. The aerosols formed in the flow were detected through Mie scattering of a 355nm laser beam. The temperature distribution of the flow was measured by molecular Rayleigh scattering thermometry. From the temperature where nucleation occurred, it was possible to identify the aerosols formed. Depending on the potassium speciation in the inlet and the presence of SO₂, they consisted of K₂SO₄, KCl, or K₂CO₃, respectively. The experiments showed that KOH was sulphated more readily than KCl, resulting in larger quantities of aerosols. The sulfation process in the counter-flow setup was simulated using a chemical kinetic model including a detailed subset for the Cl/S/K chemistry. Similar to the experimental results, much more potassium sulfate was predicted when seeding KOH compared to seeding KCl. For both KOH and KCl, sulfation was predicted to occur primarily through the reactions among atomic K, O₂ and SO₂, forming KHSO₄ and K₂SO₄. The higher propensity for sulfation of KOH compared to KCl was mostly attributed to the lower thermal stability of KOH, facilitating formation of atomic K.

According to the model, sulfation also happened through SO₃, especially for KCl (KCl→KSO₃→K₂SO₄).

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Lund University
Authors: Weng, W. (Ekstern), chen, S. (Ekstern), Wu, H. (Intern), Glarborg, P. (Intern), Li, Z. (Ekstern)
Pages: 461-468
Publication date: 2018
Optimization of Grignard Addition to Esters: Kinetic and Mechanistic Study of Model Phthalide using Flow Chemistry

The kinetics of sequential addition of a distinct Grignard species onto a lactone is studied by flow chemistry. The experimental data are shown to be consistent with a kinetic model based on four reaction steps, reaction of ester to magnesium hemiacetal, rearrangement to ketone (forward and backward) and reaction of ketone to tertiary alcohol upon quenching. The experimental derived reaction mechanism is supported by ab initio molecular computations, and the predicted activation energy is in good agreement with the experimental observations. The Grignard reaction follows a substrate-independent, reductive [2+2] cycloaddition of the Meisenheimer/Casper type. Moreover, the rearrangement equilibrium between magnesium hemiacetal and ketone is characterized and found to be feasible. Monoaddition of the ester carbonyl group is demonstrated for fluorophenyl magnesium bromide, but at reaction conditions at -40 °C with several hours of residence time. Working under cryogenic temperature conditions is essential to realizing monoaddition of the ester carbonyl group with Grignard reagents.

General information

State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Massachusetts Institute of Technology, H. Lundbeck A/S
Authors: Pedersen, M. J. (Intern), Born, S. (Ekstern), Neuenschwander, U. (Ekstern), Skovby, T. (Ekstern), Mealy, M. J. (Ekstern), Kill, S. (Intern), Dam-Johansen, K. (Intern), Jensen, K. F. (Ekstern)
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Journal: Industrial & Engineering Chemistry Research
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Organic carbon recovery modeling for a rotating belt filter and its impact assessment on a plant-wide scale

In this study, we perform a systematic plant-wide assessment of the organic carbon recovery concept on wastewater treatment plants by an advanced cellulose recovery enabling technology called rotating belt filter (RBF). To this end, first, an empirical model is developed to describe organic carbon recovery by the RBF, which is then used for the plant-wide performance evaluation to further understand the impact of organic carbon recovery by framing four different scenarios. The key features of the scenario analysis are: (i) an RBF operating with thick mat increases methane production (around 10 %) and brings down aeration energy demand (by 8 %) compared to the primary clarifier (PC) and, (ii) the sludge retention time (SRT) of the activated sludge (AS) tank increases by 55 % when an RBF runs with thick mat and therefore promotes higher nitrification rate, (iii) organic carbon recovery by the RBF does not increase the greenhouse gas (N2ON2O) emission. Further sensitivity analysis indicates that the impact of the organic carbon recovery concept depends on the wastewater characteristics, especially the cellulose content and its biodegradability. Overall, the organic carbon recovery technology can be used to provide plant specific improvements achieved by maximizing organic carbon recovery in the form of methane gas or enhancing nitrogen removal depending on the treatment plant operation objectives and priorities.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Trojan Technologies
Authors: Behera, C. R. (Intern), Santoro, D. (Ekstern), Gernaey, K. V. (Intern), Sin, G. (Intern)
Pages: 1965-1976
Publication date: 2018
Main Research Area: Technical/natural sciences

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Journal: Chemical Engineering Journal
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Polyhydroxyalkanoates (PHA) production from fermented crude glycerol: Study on the conversion of 1,3-propanediol to PHA in mixed microbial consortia

Crude glycerol, a by-product from the biodiesel industry, can be converted by mixed microbial consortia into 1,3-propanediol (1,3-PDO) and volatile fatty acids. In this study, further conversion of these main products into polyhydroxyalkanoates (PHA) was investigated with the focus on 1,3-PDO. Two different approaches for the enrichment of PHA accumulating microbial consortia using an aerobic dynamic feeding strategy were applied. With the first approach, where nitrogen was present during the whole cycle, no net production of PHA from 1,3-PDO was observed in the fermented effluent, not even in a nitrogen-limited PHA accumulation assay. Nevertheless, experiments in synthetic substrates revealed that the conversion of 1,3-PDO to PHA was possible under nitrogen limiting conditions. Thus, a different enrichment strategy was formulated where nitrogen was limited during the famine phase to stimulate the storage response. Nitrogen was still supplied during the famine phase. With the latter strategy, a net production of PHA from 1,3-PDO was observed at a yield of 0.24 Cmol PHA/Cmol 1,3-PDO. The overall yield from the fermented effluent was 0.42 Cmol PHA/Cmol substrate. Overall, the PHA yield from 1,3-PDO seemed to be limited, similarly to when using glycerol as a substrate, by a decarboxylation step and accumulation of other storage polymers such as glycogen, and possibly, lipid
inclusions.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, The Danish Polymer Centre, PILOT PLANT, SINTEF
Authors: Burniol Figols, A. (Intern), Varrone, C. (Intern), Daugaard, A. E. (Intern), Le, S. B. (Ekstern), Skiadas, I. V. (Intern), Gavala, H. N. (Intern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.49 SJR 2.629 SNIP 2.558
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.689 SNIP 2.507 CiteScore 6.63
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.957 SNIP 2.727 CiteScore 6.13
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.956 SNIP 2.693 CiteScore 6.02
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.966 SNIP 2.456 CiteScore 5.15
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.867 SNIP 2.374 CiteScore 5.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.582 SNIP 2.196
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.319 SNIP 2.225
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.065 SNIP 2.19
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.994 SNIP 2.208
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.895 SNIP 2.214
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.114 SNIP 2.337
Potassium Capture by Kaolin, Part 1: KOH

The reaction of gaseous KOH with kaolin and mullite powder under suspension-fired conditions was studied by entrained flow reactor (EFR) experiments. A water-based slurry containing kaolin/mullite and KOH was fed into the reactor and the reacted solid samples were analyzed to quantify the K-capture level. The effect of reaction temperature, K-concentration in the flue gas, and, thereby, molar ratio of K/(Al+Si) in reactants, gas residence time, and solid particle size on K-capture reaction was systematically investigated. Corresponding equilibrium calculations were conducted with FactSage 7.0. The experimental results showed that kaolin reached almost full conversion to K-aluminosilicates under suspension-fired conditions at 1100–1450 °C for a residence time of 1.2 s and a particle size of D50 = 5.47 μm. The amount of potassium captured by kaolin generally followed the equilibrium at temperatures above 1100°C, but lower conversion was observed at 800 and 900 °C. Crystalline kaliophilite (KAlSiO4) was formed at higher temperatures (1300 and 1450 °C), whereas, amorphous K-aluminosilicate was formed at lower temperatures. Coarse kaolin (D50 = 13.48 μm) captured KOH less effectively than normal (D50 = 5.47 μm) and fine (D50 = 3.51 μm) kaolin powder at 1100 and 1300 °C. The difference was less significant at 900°C. Mullite generated from kaolin captured KOH less effectively than kaolin at temperatures below 1100 °C. However, at 1300 and 1450 °C, the amount of potassium captured by mullite became comparable to that of kaolin.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Ørsted Bioenergy & Thermal Power
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Potassium Capture by Kaolin, Part 2: K₂CO₃, KCl, and K₂SO₄

The reaction of kaolin powder with K₂CO₃, KCl, and K₂SO₄ under suspension-fired conditions was studied by entrained flow reactor experiments and equilibrium calculations. The influence of reaction temperature, K-concentration in the flue gas, molar ratio of K/(Al + Si) in the reactants, and gas residence time on the reaction was investigated. The results showed that the K-capture level (Cₖ) (g potassium reacted by per g kaolin available) of K₂CO₃ and KCl by kaolin generally followed the equilibrium predictions at temperatures above 1100 °C, when using a kaolin particle size of D₅₀ = 5.47 μm and a residence time of 1.2 s. This revealed that a nearly full conversion was obtained without kinetic or transport limitations at the conditions applied. At 800 and 900°C, the measured conversions were lower than the equilibrium predictions, indicating that the reactions were either kinetically or diffusion controlled. The measured Cₖ of K₂SO₄ by kaolin was much lower than the equilibrium predictions. Kaliophilite (KAlSiO₄) product was predicted by the equilibrium calculations of the K₂SO₄ capture reaction; however the XRD results revealed that leucite (KAl(Si₂O₆)) was formed. Compared with the Cₖ of KOH reacting with kaolin, the Cₖ of K₂CO₃ was similar, while the Cₖ values of KCl and K₂SO₄ were both lower.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Ørsted Bioenergy & Thermal Power
Pages: 3566-3578
Prediction of acid dissociation constants of organic compounds using group contribution methods

In this paper, group contribution (GC) property models for the estimation of acid dissociation constants (Ka) of organic compounds are presented. Three GC models are developed to predict the negative logarithm of the acid dissociation constant $pK_a$: (a) a linear GC model for amino acids using 180 data-points with average absolute error of 0.23; (b) a non-linear GC model for organic compounds using 1622 data-points with average absolute error of 1.18; (c) an artificial neural network (ANN) based GC model for the organic compounds with average absolute error of 0.17. For each of the developed model, uncertainty estimates for the predicted $pK_a$ values are also provided. The model details, regressed parameters and application examples are highlighted.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CERE – Center for Energy Resources Engineering, Technical University of Denmark, Max Planck Institute for Dynamics of Complex Technical Systems
Authors: Zhou, T. (Ekstern), Jhamb, S. (Intern), Liang, X. (Intern), Sundmacher, K. (Ekstern), Gani, R. (Intern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.319 SNIP 1.708
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.293 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.299 SNIP 1.6
Web of Science (2008): Indexed yes
Two algorithms are proposed for isothermal multiphase flash. These are referred to as modified RAND and vol-RAND. The former uses the chemical potentials and molar-phase amounts as the iteration variables, while the latter uses chemical potentials and phase volumes to cosolve a pressure-explicit equation of state (EOS) with the equilibrium equations. Compared with the conventional secondorder approach using Gibbs-energy minimization, these methods are more structured, with all components in all phases treated in the same way. Both have been derived to include chemical reactions for any number of phases along with the possible simplifications for only phase equilibria. The simple structured implementation of these methods is demonstrated for modified RAND and vol-RAND. The rate of convergence of the methods presented is shown to be the same as the conventional second-order method for isothermal flash. It is demonstrated that the use of an association term [cubic plus association (CPA)] adds little additional computational cost when using vol-RAND compared with a simple cubic Soave-Redlich-Kwong (SRK) without association. The RAND methods scale better in terms of the $O(n^3)$ operations as more phases are introduced, and are computationally less expensive than the conventional Gibbs minimization method for more than three phases.

RAND-Based Formulations for Isothermal Multiphase Flash

General information
State: Accepted/In press
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering
Authors: Paterson, D. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)
Number of pages: 15
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.01 SJR 0.95 SNIP 2.003
Web of Science (2016): Indexed yes
Redesign of a Grignard-Based Active Pharmaceutical Ingredient (API) Batch Synthesis to a Flow Process for the Preparation of Melitracen HCl

A Grignard-based batch process, for the preparation of Melitracen HCl, has been redesigned to fit a continuous reactor system. The Grignard addition is carried out at room temperature, with subsequent hydrolysis of the magnesium alkoxide intermediate followed by dehydration of the resulting alcohol. The product undergoes further workup by simple gravimetric phase separation and then crystallization with 2 M HCl in diethyl ether to afford pure Melitracen HCl. All steps in the laboratory setup were concatenated, and the setup was proven capable of producing a significant portion of the commercial quantities of Melitracen HCl. The flow setup profits from a reduced footprint, lower energy consumption, fewer synthetic steps, and reduced raw material usage compared to the batch process.
Reversible and irreversible deactivation of Cu-CHA NH₃-SCR catalysts by SO₂ and SO₃

Abstract
Sulfur oxides are a common source for the deactivation of Cu-exchanged CHA zeolite based catalysts used for NOx reduction in diesel exhausts by selective catalytic reduction with NH₃ (NH₃-SCR). Since water and possible formation of SO₃ affect the deactivation of Cu-CHA catalysts, the deactivation in the presence of SO₂ or a mixture of SO₂ and SO₃ was studied by measuring the SCR activity in wet and dry gas at 200 and 550 °C. The estimated S-content in the catalysts before and after 4 h regeneration at 550 °C in NO, NH₃, O₂ and H₂O was related to the deactivation. The deactivation can be divided into two parts: a reversible deactivation that is restored by the regeneration treatment, and an irreversible part. The irreversible deactivation does not affect the activation energy for NH₃-SCR and display a 1:1 correlation with the S-content, consistent with deactivation by Cu-sulfate formation. The reversible deactivation results in a lower activation energy and a deactivation that is larger than expected from the S-content. The presence of SO₃ at 200 °C leads to higher reversible and irreversible deactivation, but has no significant impact at 550 °C. Furthermore, the irreversible deactivation is always higher when exposed at 200 °C than at 550 °C, and in wet conditions, compared to a dry feed. The deactivation is predominantly reversible, making regeneration at 550 °C a realistic approach to handle S-poisoning in exhaust systems.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Houston, Haldor Topsoe AS
Authors: Hammershøi, P. S. (Intern), Jangjou, Y. (Ekstern), Epling, W. S. (Ekstern), Jensen, A. D. (Intern), Janssens, T. V. (Ekstern)
Pages: 38–45
Publication date: 2018
Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 8.86 SJR 2.583 SNIP 2.12
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.26 SNIP 2.081 CiteScore 7.72
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.232 SNIP 2.164 CiteScore 6.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.345 SNIP 2.134 CiteScore 6.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.629 SNIP 2.236 CiteScore 6.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Role of Biocatalysis in Sustainable Chemistry

Based on the principles and metrics of green chemistry and sustainable development, biocatalysis is both a green and sustainable technology. This is largely a result of the spectacular advances in molecular biology and biotechnology achieved in the past two decades. Protein engineering has enabled the optimization of existing enzymes and the invention of entirely new biocatalytic reactions that were previously unknown in Nature. It is now eminently feasible to develop enzymatic transformations to fit predefined parameters, resulting in processes that are truly sustainable by design. This approach has successfully been applied, for example, in the industrial synthesis of active pharmaceutical ingredients. In addition to the use of protein engineering, other aspects of biocatalysis engineering, such as substrate, medium, and reactor engineering, can be utilized to improve the efficiency and cost-effectiveness and, hence, the sustainability of biocatalytic reactions. Furthermore, immobilization of an enzyme can improve its stability and enable its reuse multiple times, resulting in better performance and commercial viability. Consequently, biocatalysis is being widely applied in the production of pharmaceuticals and some commodity chemicals. Moreover, its broader application will be further stimulated in the future by the emerging biobased economy.
Room-temperature solid phase ionic liquid (RTSPIL) coated ω-transaminases: Development and application in organic solvents

ω-Transaminases ATA-40, ATA-47 and ATA-82P were coated with room-temperature solid phase ionic liquids (RTSPILs) by means of three methods, melt coating, precipitation coating, and co-lyophilization, and showed increased stability in all
of the five tested organic solvents. Co-lyophilization and melt coating were further found to have an activating effect on the enzymes. The former led to an up to 8-fold increase of reaction rate and excellent recyclability. The coating also protected the cofactor pyridoxal 5'-phosphate (PLP), which is essential for transaminase activity, from degradation, leading to a reaction proceeding for 27 days. With this method the sparingly water soluble substrate 5-bromo-1-indenone could be processed enzymatically in cyclohexane as solvent.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium, Graz University of Technology, Solvionic, Espagne
Authors: Grabner, B. (Ekstern), Nazario, M. A. (Ekstern), Gundersen, M. T. (Intern), Loïs, S. (Ekstern), Fantini, S. (Ekstern), Bartsch, S. (Ekstern), Woodley, J. M. (Intern), Gruber-Woelfler, H. (Ekstern)
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**Publication information**

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Volume: 452
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Source: FindIt
Source-ID: 2398202771
Publication: Research - peer-review › Journal article – Annual report year: 2018

Simple preparation of thiol-ene particles in glycerol and surface functionalization by thiol-ene chemistry (TEC) and surface chain transfer free radical polymerization (SCT-FRP)

Thiol-ene (TE) based polymer particles have traditionally been prepared via emulsion polymerization in water (using surfactants, stabilizers and co-solvents). Here, we present a green and simple alternative with excellent control over particle size, while avoiding the addition of stabilizers. Glycerol is applied as a dispersing medium for the preparation of offstoichiometric TE (OSTE) microparticles, where sizes in the range of 40 to 400 µm are obtained solely by changing the mixing speed of the emulsions prior to cross-linking. Control over surface chemistry is achieved by surface functionalization of excess thiol groups via photochemical thiol-ene chemistry (TEC) resulting in a functional monolayer. In addition, surface chain transfer free radical polymerization (SCT-FRP) was used for the first time to introduce a thicker polymer layer on the particle surface. The application potential of the system is demonstrated by using functional particles as a support for immobilized enzymes in a continuous plug-flow reactor.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for BioProcess Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre
Authors: Hoffmann, C. (Intern), Chiaula, V. (Intern), Pinelo, M. (Intern), Woodley, J. (Intern), Daugaard, A. E. (Intern)
Number of pages: 28
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Scopus rating (2016): CiteScore 4.19 SJR 1.689 SNIP 0.946
Web of Science (2016): Indexed yes
Handling acidic chemicals is a challenge in the chemical industry, requiring a careful choice of contact material. Certain thermoset organic coatings are applicable in low pH environments, but when particulate erosion is also present the performance demand is increased. This is the case in, e.g., stirred tanks for agitated leaching of copper ore, where sulfuric acid is mixed with an erosive slurry. A pilot-scale agitated leaching tank was designed and constructed to explore the performance of selected thermoset coatings in such an environment. For reference, simple immersion experiments were conducted. Coating durability was estimated by observing the film thickness change during exposure. It was found to be a function of film swelling and film contraction, due to chemical exposure, as well as the “polishing” caused by erosive wear. Film reduction rates varied with radial position in the tank bottom-placed coating samples. Maximum rates were found about halfway between the reactor center and wall. Polishing rates also varied significantly with acid concentration, most likely due to chemical reactions taking place between the acid and the coatings, damaging surface mechanical properties, similar to the erosion/corrosion-type phenomena found in metals. A vinyl ester-based coating was the most resistant to the simultaneous erosive/acidic exposure, with a maximum polishing rate of 3.24±0.61 μm/week, while novolac epoxy and polyurethane coatings showed high polishing rates of 11.7±0.150 and 13.4±0.57μm/week, respectively.

**General information**

State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, The Hempel Foundation Coatings Science and Technology Centre (CoaST), CHEC Research Centre, Hempel AS
Structure, computational and biochemical analysis of PcCel45A endoglucanase from *Phanerochaete chrysosporium* and catalytic mechanisms of GH45 subfamily C members

The glycoside hydrolase family 45 (GH45) of carbohydrate modifying enzymes is mostly comprised of β-1,4-endoglucanases. Significant diversity between the GH45 members has prompted the division of this family into three subfamilies: A, B and C, which may differ in terms of the mechanism, general architecture, substrate binding and cleavage. Here, we use a combination of X-ray crystallography, bioinformatics, enzymatic assays, molecular dynamics simulations and site-directed mutagenesis experiments to characterize the structure, substrate binding and enzymatic specificity of the GH45 subfamily C endoglucanase from *Phanerochaete chrysosporium* (PcCel45A). We investigated the role played by different residues in the binding of the enzyme to cellulose oligomers of different lengths and examined the
structural characteristics and dynamics of *PcCel45A* that make subfamily C so dissimilar to other members of the GH45 family. Due to the structural similarity shared between *PcCel45A* and domain I of expansins, comparative analysis of their substrate binding was also carried out. Our bioinformatics sequence analyses revealed that the hydrolysis mechanisms in GH45 subfamily C is not restricted to use of the imidic asparagine as a general base in the “Newton’s cradle” catalytic mechanism recently proposed for this subfamily.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, University of São Paulo, University of Campinas, Centro de Tecnologia Canavieira
Authors: Godoy, A. S. (Ekstern), Pereira, C. S. (Ekstern), Ramia, M. P. (Ekstern), Silveira, R. L. (Ekstern), Camilo, C. M. (Ekstern), Kadowaki, M. A. (Ekstern), Lange, L. (Intern), Busk, P. K. (Intern), Nascimento, A. S. (Ekstern), Skaf, M. S. (Ekstern), Polikarpov, I. (Ekstern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.63 SJR 1.625 SNIP 1.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.057 SNIP 1.684 CiteScore 5.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.103 SNIP 1.544 CiteScore 4.75
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.886 SNIP 1.51 CiteScore 4.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.458 SNIP 0.896 CiteScore 2.44
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
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Structure_computational.pdf
DOIs:
10.1038/s41598-018-21798-9
Source: FindIt
Source-ID: 2396646140
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**Substrate specificity and transfucosylation activity of GH29 α-l-fucosidases for enzymatic production of human milk oligosaccharides**
Abstract Human milk oligosaccharides (HMOs) constitute a unique family of bioactive lactose-based molecules present in human breast milk. HMOs are of major importance for infant health and development but also virtually absent from bovine milk used for infant formula. Among the HMOs, the fucosylated species are the most abundant. Transfucosylation catalysed by retaining α-l-fucosidases is a new route for manufacturing biomimetic HMOs. Seven α-l-fucosidases from glycosyl hydrolase family 29 were expressed, characterized in terms of substrate specificity and thermal stability, and
shown to be able to catalyse transfucosylation. The α-l-1,3/4-fucosidase CpAfc2 from Clostridium perfringens efficiently catalysed the formation of the more complex human milk oligosaccharide structure lacto-N-fucopentaose II (LNFP II) using 3-fucosyllactose as fucosyl donor and lacto-N-tetraose as acceptor with a 39% yield. α-l-Fucosidases FgFCO1 from Fusarium graminearum and Mfuc5 from a soil metagenome were able to catalyse transfucosylation of lactose using citrus xylloglucan as fucosyl donor. FgFCO1 catalysed formation of 2′-fucosyllactose, whereas Mfuc5 catalysis mainly produced an unidentified, non-HMO fucosyllactose, reaching molar yields based on the donor substrate of 14% and 18%, respectively.

**General information**

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*Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Technical University of Denmark*


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*BFI (2016): BFI-level 1*

*Scopus rating (2016): CiteScore 3.67 SJR 1.065 SNIP 1.269*

*Web of Science (2016): Indexed yes*

*BFI (2015): BFI-level 1*

*Scopus rating (2015): SJR 1.069 SNIP 1.07 CiteScore 3.07*

*Web of Science (2015): Indexed yes*

*BFI (2014): BFI-level 1*

*Scopus rating (2014): SJR 0.994 SNIP 1.248 CiteScore 2.77*

*Web of Science (2014): Indexed yes*

*BFI (2013): BFI-level 1*

*Scopus rating (2013): SJR 0.819 SNIP 0.988 CiteScore 2.5*

*ISI indexed (2013): ISI indexed yes*

*BFI (2012): BFI-level 1*

*Scopus rating (2012): SJR 0.788 SNIP 0.836 CiteScore 2.12*

*ISI indexed (2012): ISI indexed yes*

*Web of Science (2012): Indexed yes*

*BFI (2011): BFI-level 1*

*Scopus rating (2011): SJR 0.934 SNIP 0.952 CiteScore 2.13*

*ISI indexed (2011): ISI indexed yes*

*Web of Science (2011): Indexed yes*

*BFI (2010): BFI-level 1*

*Scopus rating (2010): SJR 0.89 SNIP 1.023*

*BFI (2009): BFI-level 1*

*Scopus rating (2009): SJR 1.028 SNIP 1.401*

*BFI (2008): BFI-level 1*

*Scopus rating (2008): SJR 0.936 SNIP 1.098*

*Scopus rating (2007): SJR 1.381 SNIP 1.325*

*Scopus rating (2006): SJR 0.752 SNIP 0.898*

*Scopus rating (2005): SJR 0.685 SNIP 1.097*

*Scopus rating (2004): SJR 0.72 SNIP 1.043*

*Scopus rating (2003): SJR 0.626 SNIP 0.938*
Surface modification of polysulfone membranes applied for a membrane reactor with immobilized alcohol dehydrogenase

Commercially available polysulfone (PSf) membranes with a polypropylene backing are used across a broad range of applications. However, the natural properties of the PSf surface sometimes limit their application. Here we present, how the surface of supported membranes can be heterogeneously activated by lithiation followed by functionalization with acid chlorides at 0°C, permitting modification of commercial PSf membranes without compromising the mechanical integrity of the membrane. Post-functionalization polymer grafting was illustrated through both, a “grafting from” approach by surface initiated atom transfer radical polymerization (SI-ATRP) and by a “grafting to” approach exploiting Cu(I) catalyzed 1,3-cycloadditions of alkynes with azides (CuAAC) introducing hydrophilic polymers onto the membrane surface. Poly(1-vinyl imidazole) (pVim) grafted membranes were exploited as support for immobilization of alcohol dehydrogenase (ADH) in a biocatalytic membrane reactor (BMR) and demonstrated substantial improvements in terms of operational enzyme stability compared to immobilization onto pristine membranes.

General information

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for BioProcess Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre
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Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information

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Ratings:
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Scopus rating (2016): CiteScore 1.38 SJR 0.395 SNIP 0.718
Scopus rating (2015): SJR 0.137 SNIP 0.142 CiteScore 0.8
Original language: English
Materials Science (all), Mechanics of Materials, Materials Chemistry, Enzyme immobilization, Polysulfone membrane, Surface functionalization
DOIs:
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Publication: Research - peer-review › Journal article – Annual report year: 2018

Syngas biomethanation: state-of-the-art review and perspectives

Significant research efforts are currently being made worldwide to develop more efficient biomethane production processes from a variety of waste streams. The biomethanation of biomass-derived syngas can contribute to increasing the potential of methane production as it opens the way for the conversion of recalcitrant biomasses, generally not fully exploitable by anaerobic digestion systems. Additionally, this biological process presents several advantages over its analogous process of catalytic methanation such as the use of inexpensive biocatalysts, milder operational conditions, higher tolerance to the impurities of syngas, and higher product selectivity. However, there are still several challenges to be addressed for this technology to reach commercial stage. This work reviews the progress made over the last few years in syngas biomethanation processes in order to provide an overview of the current state of the art of this technology. The most relevant aspects determining the performance of syngas biomethanation processes are extensively discussed here, including microbial diversity and metabolic interactions in mixed microbial consortia, the influence of operating parameters and bioreactor designs, and the potential of modelling as a tool for the design and control of this bioprocess. © 2017 Society of Chemical Industry and John Wiley & Sons, Ltd
Industrial use of lipids has been increasing as a consequence of increased developments related to biobased economies. In addition to applications in food-products, lipids are used by many industrial sectors, for example, biodiesel, edible oil, health, and personal care. Phase equilibria predictions for chemical systems with lipids play a major role in process–product modelling, simulation and design. Due to the large number of lipid-compounds involved, predictive methods like group contribution based methods are particularly suitable for estimation of pure compound and mixture properties that may not be available. Limited experimental data availability and poor performances of currently available group contribution based methods is therefore an obstacle for obtaining the necessary information regarding phase equilibria of chemical systems with lipids. In this paper, a systematic identification-regression method (to be called
identification method) for phase equilibrium modelling, where, based on the available experimentally measured phase equilibrium data, the selected model parameters are estimated in a hierarchical and efficient manner, is presented. The aim of the method is to improve the quality of phase equilibria prediction for the selected group contribution based methods. By applying the identification method, a new set of binary group interaction parameters regressed from vapour-liquid equilibrium data for chemical systems with lipids is presented for the Original UNIFAC model, together with regression statistics and model performance. An extended and updated version of the in-house SPEED Lipids database, which is used for the needed pure compound properties and phase equilibria data, is also presented.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre, CERE – Center for Energy Resources Engineering, Alfa Laval Copenhagen A/S
Authors: Perederic, O. A. (Intern), Cunico, L. P. (Intern), Kalakul, S. (Intern), Sarup, B. (Ekstern), Woodley, J. M. (Intern), Kontogeorgis, G. M. (Intern), Gani, R. (Intern)
Pages: 153-169
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Main Research Area: Technical/natural sciences

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- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.64 SJR 1 SNIP 1.163
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.075 SNIP 1.091 CiteScore 2.29
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.224 SNIP 1.306 CiteScore 2.59
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.252 SNIP 1.25 CiteScore 2.42
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.221 SNIP 1.181 CiteScore 2.41
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.24 SNIP 1.307 CiteScore 2.44
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.218 SNIP 1.462
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.116 SNIP 1.355
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.414 SNIP 1.269
- Scopus rating (2007): SJR 1.264 SNIP 1.176
- Scopus rating (2006): SJR 1.116 SNIP 1.415
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 0.913 SNIP 1.277

An integrated optimization-based framework for product and process design is proposed. The framework uses a set of methods and tools to obtain the optimal product–process design solution given a set of economic and environmental sustainability targets. The methods and tools required are property prediction through group contributions, unless supported with a database, computer-aided molecular and mixture/blend design for generation of novel as well as existing products and mathematical programming for formulating and solving multiscale integrated process–product design problems. The application of the framework is demonstrated through three case studies: (i) refrigeration cycle unit for R134a replacement, (ii) a mixed working fluid design problem for R134a replacement, and (iii) pure solvent design for water-acetic acid LLE extraction. Through the application of the framework it is demonstrated that all solutions satisfy product, process, economic, and environmental targets simultaneously. The solution is obtained through a direct deterministic mathematical optimization strategy. The framework proposed in this work is generic and can be applied to a wide range of problems where an integrated solution to process-product design is beneficial.
Replacing coal with biomass in power plants is a viable option for reducing net CO₂ emissions and combating climate change. However, biomass combustion in boilers may exacerbate problems related to ash deposition and corrosion, demanding effective deposit removal. The tensile adhesion strength of model biomass ash deposits, containing mixtures of KCl, K₂SO₄, CaO, CaSO₄, and K₂Si₄O₉, has been investigated in this study. The deposits were prepared on superheater steel tubes and sintered in an oven. The superheater steel tube was cooled by air, incorporating a temperature gradient across the deposits. After sintering, the deposits were removed using an electrically controlled arm and the corresponding tensile adhesion strength was measured. The influence of the flue gas temperature (500–700 °C), steel surface temperature (500–650 °C), and deposit composition were investigated. The results revealed that increasing the flue gas temperature as well as the steel surface temperature led to a sharp increase in the tensile adhesion strength of the model deposits. The sharp increase was typically observed near the melting temperature (or deformation temperature) of the investigated model deposits. Furthermore, migration of molten/vapor species from the outer layer of the deposit to the deposit–tube interface, causing liquid-state sintering, was observed at high flue gas temperatures.
leading to an increase in the tensile adhesion strength. Varying the ash chemistry of the model deposits revealed that the melt fraction of the deposit was highly influential in determining the deposit adhesion strength. The addition of compounds that increased the melt fraction of the deposit increased the tensile adhesion strength, whereas the addition of inert compounds with a high melting point, such as CaO, decreased the tensile adhesion strength. Moreover, the results suggested that the adhesion strength of the deposits was influenced by the corrosion occurring at the deposit–tube interface.
The Debye-Hückel theory and its importance in modeling electrolyte solutions

A colleague at the Technical University of Denmark has often stated: “Life is too short for electrolytes”. Another well-known scientist in the field of molecular simulation has recently said during an international Thermodynamics conference: “All my life I have tried to keep myself away from water and electrolytes”. Sadly, what these statements correctly imply is that there are far too many unclear questions and concepts in electrolyte thermodynamics, and associated difficulties in modeling electrolyte solutions. In this work, we attempt to shed some light on some important concepts and misconceptions in electrolyte thermodynamics associated with the development of electrolyte equations of state, with emphasis on those based on the Debye-Hückel theory. Detailed mathematics is needed for some of the derivations but for brevity and in order to emphasize the principles rather than the derivations, the latter are omitted. We first discuss the peculiarities of electrolyte thermodynamics and associated modeling and continue with the derivation of the Debye-Hückel theory. The assumptions and limits of application of Debye-Hückel are discussed in particular. Next, the Born term and its significance and implications are presented in more detail. A discussion and outlook section conclude this review. Several of the statements in this work challenge “accepted beliefs” in electrolyte thermodynamics and, while we believe that this challenge is justified, we hope that a useful debate can result in improved and predictive thermodynamic models for electrolyte solutions.
The Global Acetylome of the Human Pathogen Vibrio cholerae V52 Reveals Lysine Acetylation of Major Transcriptional Regulators

Protein lysine acetylation is recognized as an important reversible post translational modification in all domains of life. While its primary roles appear to reside in metabolic processes, lysine acetylation has also been implicated in regulating pathogenesis in bacteria. Several global lysine acetylome analyses have been carried out in various bacteria, but thus far there have been no reports of lysine acetylation taking place in the important human pathogen Vibrio cholerae. In this study, we analyzed the lysine acetylproteome of the human pathogen V. cholerae V52. By applying a combination of immuno-enrichment of acetylated peptides and high resolution mass spectrometry, we identified 3,402 acetylation sites on 1,240 proteins. Of the acetylated proteins, more than half were acetylated on two or more sites. As reported for other bacteria, we observed that many of the acetylated proteins were involved in metabolic and cellular processes and there was an over-representation of acetylated proteins involved in protein synthesis. Of interest, we demonstrated that many global transcription factors such as CRP, H-NS, IHF, Lrp and RpoN as well as transcription factors AphB, TcpP, and PhoB involved in direct regulation of virulence in V. cholerae were acetylated. In conclusion, this is the first global protein lysine acetylome analysis of V. cholerae and should constitute a valuable resource for in-depth studies of the impact of lysine acetylation in pathogenesis and other cellular processes.
The natural catalytic function of CuGE glucuronoyl esterase in hydrolysis of genuine lignin-carbohydrate complexes from birch

Glucuronoyl esterases belong to carbohydrate esterase family 15 and catalyze de-esterification. Their natural function is presumed to be cleavage of ester linkages in lignin-carbohydrate complexes particularly those linking lignin and glucuronoyl residues in xylans in hardwood. Here, we show for the first time a detailed product profile of aldouronic acids released from birchwood lignin by a glucuronoyl esterase from the white-rot fungus Cerrena unicolor (CuGE). CuGE releases substrate for GH10 endo-xylanase which results in significantly increased product release compared to the action of endo-xylanase alone. CuGE also releases neutral xylo-oligosaccharides that can be ascribed to the enzymes feruloyl esterase side activity as demonstrated by release of ferulic acid from insoluble wheat arabinoxylan. The data verify the enzyme's unique ability to catalyze removal of all glucuronoxylan associated with lignin and we propose that this is a direct result of enzymatic cleavage of the ester bonds connecting glucuronoxylan to lignin via 4-O-methyl glucuronoyl-ester linkages. This function appears important for the fungal organism's ability to effectively utilize all available carbohydrates in lignocellulosic substrates. In bioprocess perspectives, this enzyme is a clear candidate for polishing lignin for residual carbohydrates to achieve pure, native lignin fractions after minimal pretreatment.
Use of Electrohydrodynamic Processing for Encapsulation of Sensitive Bioactive Compounds and Applications in Food

The use of vitamins, polyphenolic antioxidants, omega-3 polyunsaturated fatty acids (PUFAs), and probiotics for the fortification of foods is increasing. However, these bioactive compounds have low stability and need to be protected to
avoid deterioration in the food system itself or in the gastrointestinal tract. For that purpose, efficient encapsulation of the compounds may be required. Spray drying is one of the most commonly used encapsulation techniques in the food industry, but it uses high temperature, which can lead to decomposition of the bioactive compounds. Recently, alternative technologies such as electrospaying and electrospinning have received increasing attention. This review presents the principles of electrohydrodynamic processes for the production of nano-microstructures (NMSs) containing bioactive compounds. It provides an overview of the current use of this technology for encapsulation of bioactive compounds and discusses the future potential of the technology. Finally, the review discusses advanced microscopy techniques to study the morphology of NMSs.

Visualization of the distribution of surface-active block copolymers in PDMS-based coatings

Poly(dimethylsiloxane) (PDMS) has been widely employed in the area of fouling-release coatings and other fields due to its unique combination of properties including low elastic modulus and low glass transition temperature. The drawback of PDMS in some applications is its hydrophobic surface, which results in non-specific protein adsorption and wettability issues. Poly(ethylene glycol)-based surface-active block copolymers and surfactants have been added to PDMS coatings and films to impart biofouling resistance and hydrophilicity to the PDMS surface with successful results. Information regarding the distribution and release of these block copolymers from PDMS-based coatings has been previously reported. However, the distribution and behaviour of these compounds in the bulk of the PDMS coating are not fully understood.

A novel fluorescent-labelled triblock PEG-b-PDMS-b-PEG copolymer was synthesized and added to a PDMS coating for visualization purposes. The surface-activity and biofouling resistance of the synthesized copolymer was confirmed by water contact angle measurements and seawater immersion experiments. Confocal laser scanning microscopy (CLSM) images showed that the triblock copolymer aggregates in spherical domains within the PDMS coating film. The size of these domains vary between 1 and 7 μm, with larger domains being present on the bulk of the film and smaller closer to the surface. The diffusion of the copolymer could be observed over time, with copolymer molecules diffusing from the bulk to the surfaces of the PDMS film. Finally, an overview of the possibilities provided by the presented methodology in the field of fouling-release coatings is discussed.
What has happened to the "aquatic phycocymetes" (sensu Sparrow)? Part I: A brief historical perspective

Abstract The "aquatic phycocymetes" constitute an ecologically and economically important assemblage of eukaryotic microorganisms, because they share many morphological traits and important ecological functions and they interact with each other in aquatic ecosystems. The last two decades of research have provided both molecular and structural evidence that the "aquatic phycocymetes" are a diverse, polyphyletic grouping and therefore not a valid taxonomic entity. Very little research has been conducted for many years with the "aquatic phycocymetes", possibly because in general these microorganisms are often hard to isolate and maintain in most laboratory facilities, little background data has been available to identify the species, the studies were time consuming, the state of the art technology in many cases did not permit studies on these groups and they were thought to be economically and ecologically unimportant. However, this perception has changed recently. For example, some of these species (1) are now known to play important roles in biomass conversion and sequestration of CO2, (2) are parasites of many fungal, plant and animal species, (3) may harbor genes of important enzymes for industrial applications and (4) can serve as indicator species for eco-tox monitoring. This review discusses the assemblages of microorganisms which Sparrow placed into the aquatic phycocymetes, their history in brief and their current phylogenetic placement.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, University of Sydney, Instituto de Botanica de Sao Paulo
Authors: Gleason, F. H. (Ekstern), Marano, A. V. (Ekstern), Lilje, O. (Ekstern), Lange, L. (Intern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.422 SNIP 1.728 CiteScore 5.32
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.754 SNIP 1.227 CiteScore 4
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ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.343 SNIP 1.334 CiteScore 3.45
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.922 SNIP 1.101 CiteScore 2.58
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.982 SNIP 1.519
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.817 SNIP 1.467
What has happened to the "aquatic phycomycetes" (sensu Sparrow)? Part II: Shared properties of zoosporic true fungi and fungus-like microorganisms

Many species of zoosporic heterotrophic parasites, saprotrophs and mutualists in the Phyla Perkinsozoa (dinoflagellates), Oomycota, Hyphochytriomycota, Labyrinthulomycota and Phyomyxea share morphological characteristics with zoosporic true fungi especially with some of the Chytridiomycota and with fungus-like organisms in the Phyla Mesomycetozoea, Chytridiomycota and Aphelidae. These characteristics include chemotactic motile zoospores, zoosporangia which produce zoospores, thick walled resistant cysts, rhizoid-like structures, hyphal-like structures and cell walls surrounding the cells in several phases of their life cycle. These assemblages also inhabit both marine and freshwater ecosystems in which aquatic fungi and fungus-like organisms are found, have similar life cycles, grow on similar substrates, use similar infection strategies and infect some of the same host plants and animals. Many of these species were once included in the aquatic phycomycetes, an ecological assemblage of microorganisms but not a valid taxonomic group. Some of the shared characteristics are discussed in this review.
Wood pellet milling tests in a suspension-fired power plant

This paper investigates the milling behavior of two industrial wood pellet qualities (designated I1 and I2 as per ISO 17225-2:2014) in large-scale coal roller mills, each equipped with a dynamic classifier. The purpose of the study was to test if pellet comminution and subsequent particle classification (i.e., the classifier cut size) are affected by the internal pellet particle size distribution obtained after pellet disintegration in hot water. Furthermore, optimal conditions for comminuting pellets were identified. The milling behavior was assessed by determining the specific grinding energy consumption and the differential mill pressure. The size and shape of comminuted pellets sampled from burner pipes were analyzed by dynamic image analysis and sieve analysis, respectively. The results showed that the internal pellet particle size distribution affected both the milling behavior and the classifier cut size. I2 pellets with coarser internal particles than I1 pellets required more energy for milling, led to a higher mill pressure drop and showed a larger classifier cut size. Comminuted pellet particles sampled from burner pipes were notably finer than internal pellet (feed) particles. At similar mill-classifier conditions, characteristic particle sizes of 0.50mm for comminuted I1 pellets (compared to 0.83mm for material within I1 pellets) and of 0.56mm for comminuted I2 pellets (compared to 1.09mm for material within I2 pellets), respectively, were obtained. Pellet comminution at lower mill loads and lower primary airflow rates reduced the mill power consumption, the mill pressure drop, and the classifier cut size. However, this was at the expense of a higher specific grinding energy consumption. Derived 2D shape parameters for comminuted and internal pellet particles were similar. Mill operating changes had a negligible effect on the original elongated wood particle shape. To achieve the desired comminuted product fineness (i.e., the classifier cut size) with lower specific grinding energy consumption, power plant operators need to choose pellets with a finer internal particle size distribution.

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  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): SJR 1.519 SNIP 1.822 CiteScore 4.09
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 1.629 SNIP 2.161 CiteScore 3.96
  BFI (2013): BFI-level 2
  Scopus rating (2013): SJR 1.636 SNIP 2.142 CiteScore 3.83
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 2
  Scopus rating (2012): SJR 1.682 SNIP 2.075 CiteScore 3.77
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  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 2
  Scopus rating (2011): SJR 1.575 SNIP 1.773 CiteScore 3.38
  ISI indexed (2011): ISI indexed yes
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  Scopus rating (2010): SJR 1.629 SNIP 1.88
  Web of Science (2010): Indexed yes
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  Scopus rating (2009): SJR 1.545 SNIP 1.856
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  BFI (2008): BFI-level 1
  Scopus rating (2008): SJR 1.471 SNIP 1.718
  Web of Science (2008): Indexed yes
  Scopus rating (2007): SJR 1.226 SNIP 1.654
  Web of Science (2007): Indexed yes
  Scopus rating (2006): SJR 0.986 SNIP 1.404
  Scopus rating (2005): SJR 0.751 SNIP 1.143
  Web of Science (2005): Indexed yes
  Scopus rating (2004): SJR 0.82 SNIP 1.142
  Scopus rating (2003): SJR 0.941 SNIP 1.134
  Scopus rating (2002): SJR 0.731 SNIP 1.12
  Scopus rating (2001): SJR 0.611 SNIP 0.992
  Scopus rating (2000): SJR 0.429 SNIP 0.967
  Web of Science (2000): Indexed yes
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Estimation of caffeine intake from analysis of caffeine metabolites in wastewater

Caffeine metabolites in wastewater were investigated as potential biomarkers for assessing caffeine intake in a population. The main human urinary metabolites of caffeine were measured in the urban wastewater of ten European cities and the metabolic profiles in wastewater were compared with the human urinary excretion profile. A good match was found for 1,7-dimethyluric acid, an exclusive caffeine metabolite, suggesting that might be a suitable biomarker in wastewater for assessing population-level caffeine consumption. A correction factor was developed considering the percentage of excretion of this metabolite in humans, according to published pharmacokinetic studies. Daily caffeine intake estimated from wastewater analysis was compared with the average daily intake calculated from the average amount of coffee consumed by country per capita. Good agreement was found in some cities but further information is needed to standardize this approach. Wastewater analysis proved useful to providing additional local information on caffeine use.

General information

State: Published
Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of South Australia, University of Oslo, University of Antwerp, Swiss Federal Institute of Aquatic Science and Technology (Eawag), Universidade do Porto, University of Queensland, University of Amsterdam, Universitat Jaume I, Istituto di Ricerche Farmacologiche Mario Negri, University of Bath, Chemical Water Quality and Health, Norwegian Institute for Water Research
Authors: Gracia-Lor, E. (Ekstern), Rousis, N. I. (Ekstern), Zuccato, E. (Ekstern), Bade, R. (Ekstern), Baz-Lomba, J. A. (Ekstern), Castrignanò, E. (Ekstern), Causanilles Llanes, A. (Ekstern), Hernández, F. (Ekstern), Kasprzyk-Hordern, B. (Ekstern), Kinyua, J. (Ekstern), McCail, A. (Ekstern), van Nuijs, A. L. N. (Ekstern), Plósz, B. G. (Intern), Ramin, P. (Intern), Ryu, Y. (Ekstern), Santos, M. M. (Ekstern), Thomas, K. V. (Ekstern), de Voogt, P. (Ekstern), Yang, Z. (Ekstern), Castiglioni, S. (Ekstern)
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.09 SJR 1.621 SNIP 1.849
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.635 SNIP 1.847 CiteScore 4.2
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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.527 SNIP 1.759 CiteScore 3.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.773 SNIP 1.811 CiteScore 3.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.798 SNIP 1.681 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
A DEVICE AND METHOD FOR MEASURING TAR IN A TAR-ENVIRONMENT

The present disclosure describes a device and corresponding method for measuring tar in a tar environment, e.g., a tar producing environment such as a stove or a combustion engine, based on UV absorption spectroscopy. A first measurement along an optical path in the tar environment is performed at a wavelength less than 340 nm at which both tar and non-tar elements absorb. This measurement is compensated for non-tar absorption by means of a second measurement at a wavelength equal to or greater than 340 nm at which tar does not absorb. From the non-tar compensated absorbance value a measure of tar in the tar environment is derived and an air intake in the tar environment is regulated based on the measure of tar.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Clausen, S. (Intern), Fateev, A. (Intern)
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17th International Conference on Petroleum Phase Behavior and Fouling
This special section of Energy & Fuels contains contributed papers from the 17th International Conference on Petroleum Phase Behavior and Fouling (Petrophase 2016). Petrophase 2016 was organized by the Technical University of Denmark and Schlumberger and took place in Elsinore (Helsingør) Denmark from June 19th to 23rd at the Beach Hotel Marienlyst. Petrophase is an international conference aimed at researchers in industry and academia dedicated to the study of the properties and chemistry of petroleum fluids and their effect on producing, processing, and refining in the upstream, midstream, and downstream industries. The conference started in 1999 as “The International Conference on Petroleum Phase Behavior & Fouling” and has since evolved into an annual event taking place in countries all around the world. Petrophase has been fortunate to have enjoyed financial and organizational support from many academic and industrial institutions through the years. Despite its growth over the years, Petrophase has always had the feel of an intimate conference where all participants are present in all of the activities.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry, Asphaltteam
Authors: von Solms, N. (Intern), Yan, W. (Intern), Andersen, S. (Ekstern)
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BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.05
ISI indexed (2011): ISI indexed yes
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Accurate particle speed prediction by improved particle speed measurement and 3-dimensional particle size and shape characterization technique

Accurate particle mass and velocity measurement is needed for interpreting test results in erosion tests of materials and coatings. The impact and damage of a surface is influenced by the kinetic energy of a particle, i.e. particle mass and velocity. Particle mass is usually determined with optical methods, e.g. laser light scattering, and velocity by the double disk (DD) method. In this article we present two novel techniques, which allow a more accurate measurement of mass, velocity and shape, and we later compare the experimentally obtained flow velocities of particles with a simulation that also includes the particle’s shape parameter, known as sphericity. Mass and sphericity are obtained from 3-dimensional data with an industrial X-ray computed tomography (CT) scanner. CT data can be used to accurately determine the volume-basis median of the particles (using the volume-equivalent particle diameter). Velocity is measured with a fast 2-dimensional particle imaging method using a pulsed LED. Good agreement of the measured and simulated particle velocity was found when including the sphericity from CT results. 2-dimensional optical particle size measurements in the jet of an erosion rig are compared with detailed 3-dimensional CT measurements and a low angle laser light scattering (LALLS) measurement system for six different samples of particles. It is shown that the particle volume or mass is usually overestimated by 16–22% when using 2-dimensional methods or LALLS. For CT allows additionally the surface-equivalent diameter to be calculated by using 2-dimensional projections of each particle, these results can be used to correct particle diameters measured with the particle imaging method using a pulsed LED.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Photonics Engineering, Physikalisch-Technische Bundesanstalt, Ricerca Sistema Energetico SpA
Authors: Cernuschi, F. (Ekstern), Rothleitner, C. (Ekstern), Clausen, S. (Intern), Neuschaefer-Rube, U. (Ekstern), Illermann, J. (Ekstern), Lorenzoni, L. (Ekstern), Guardamagna, C. (Ekstern), Larsen, H. E. (Intern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Acid-resistant organic coatings for the chemical industry: a review

Industries that work with acidic chemicals in their processes need to make choices on how to properly contain the substances and avoid rapid corrosion of equipment. Certain organic coatings and linings can be used in such environments, either to protect vulnerable construction materials, or, in combination with fiber reinforcement, to replace them. However, degradation mechanisms of organic coatings in acid service are not thoroughly understood and relevant quantitative investigations are scarce. This review describes the uses and limitations of acid-resistant coatings in the chemical industry, with a comparison to alternative resistant materials based on metals or ceramics. In addition, coating degradation phenomena, caused by acid exposure, are mapped to the extent possible, and analysis methods for detecting coating degradation type and severity are listed and discussed. It is concluded that more knowledge on chemical and physical degradation mechanisms is required, and that improvements in resistance to elevated temperatures and abrasion would decrease the risk of use and increase the potential application areas of organic coatings exposed to acidic environments in the chemical industry.
A comparative study on the activity of fungal lytic polysaccharide monooxygenases for the depolymerization of cellulose in soybean spent flakes

Lytic polysaccharide monooxygenases (LPMOs) are copper-dependent enzymes capable of the oxidative breakdown of polysaccharides. They are of industrial interest due to their ability to enhance the enzymatic depolymerization of recalcitrant substrates by glycoside hydrolases. In this paper, twenty-four lytic polysaccharide monooxygenases (LPMOs) expressed in Trichoderma reesei were evaluated for their ability to oxidize the complex polysaccharides in soybean spent flakes, an abundant and industrially relevant substrate. TrCel61A, a soy-polysaccharide-active AA9 LPMO from T. reesei, was used as a benchmark in this evaluation. In total, seven LPMOs demonstrated activity on pretreated soy spent flakes, with the products from enzymatic treatments evaluated using mass spectrometry and high performance anion exchange chromatography. The hydrolytic boosting effect of the top-performing enzymes was evaluated in combination with endoglucanase and beta-glucosidase. Two enzymes (TrCel61A and Aspte6) showed the ability to release more than 36% of the pretreated soy spent flake glucose - a greater than 75% increase over the same treatment without LPMO addition.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DuPont™ Industrial Biosciences, DuPont Nutrition Biosciences Aps
Authors: Pierce, B. (Intern), Wittrup Agger, J. (Intern), Zhang, Z. (Ekstern), Wichmann, J. (Ekstern), Meyer, A. S. (Intern)
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Scopus rating (2016): CiteScore 2.03 SJR 0.654 SNIP 0.801
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.59 SNIP 0.839 CiteScore 1.98
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.638 SNIP 0.856 CiteScore 2.01
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.639 SNIP 0.86 CiteScore 2.22
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.773 SNIP 1.017 CiteScore 2.2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.76 SNIP 1.062 CiteScore 2.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 0.722 SNIP 0.868
Web of Science (2010): Indexed yes
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A computer-aided approach for achieving sustainable process design by process intensification

Process intensification can be applied to achieve sustainable process design. In this paper, a systematic, 3-stage synthesis-intensification framework is applied to achieve more sustainable design. In stage 1, the synthesis stage, an objective function and design constraints are defined and a base case is synthesized. In stage 2, the design and analysis stage, the base case is analyzed using economic and environmental analyses to identify process hot-spots that are translated into design targets. In stage 3, the innovation design stage, phenomena-based process intensification is performed to generate flowsheet alternatives that satisfy the design targets thereby, minimizing and/or eliminating the process hot-spots. The application of the framework is highlighted through the production of para-xylene via toluene methylation where more sustainable flowsheet alternatives that consist of hybrid/intensified unit operations are generated from the application of phenomena-based process intensification.

General information
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Currently, the process industry is moving towards the design of innovative, more sustainable processes that show improvements in both economic and environmental factors. The design space of unit operations that can be combined to generate process flowsheet alternatives considering known unit operations as well as reported hybrid/intensified unit operations is large and can be difficult to manually navigate in order to determine the best process flowsheet for the production of a desired chemical product. Therefore, it is beneficial to utilize computer-aided methods and tools to enumerate, analyze and determine within the design space, the more sustainable processes. In this paper, an integrated...
computer-aided software-tool that searches the design space for hybrid/intensified more sustainable process options is presented. Embedded within the software architecture are process synthesis and intensification methods that operate at multiple scales, namely, unit operation, task and phenomena. First a base case process flowsheet (if it is not already available) is generated through process synthesis considering only known unit operations. The generated or supplied base case is then analyzed in order to identify process bottlenecks/limitations (hot-spots) that are translated into design targets. Next, phenomena-based synthesis is performed to identify process flowsheets that match the design targets through the use of hybrid/intensified unit operations. As these process flowsheets satisfy all process constraints while also matching the design targets, they are therefore more sustainable than the base case. The application of the software-tool to the production of biodiesel is presented, highlighting the main features of the computer-aided, multi-stage, multi-scale methods that are able to determine more sustainable designs.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Novo Nordisk AS, Auburn University, Technical University of Denmark  
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- Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04  
- Web of Science (2015): Indexed yes  
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- Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22  
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- BFI (2011): BFI-level 2  
- Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8  
- ISI indexed (2011): ISI indexed yes  
- Web of Science (2011): Indexed yes  
- BFI (2010): BFI-level 2  
- Scopus rating (2010): SJR 1.176 SNIP 1.796  
- Web of Science (2010): Indexed yes  
- BFI (2009): BFI-level 2  
- Scopus rating (2009): SJR 1.154 SNIP 2.166  
- Web of Science (2009): Indexed yes  
- BFI (2008): BFI-level 2  
- Scopus rating (2008): SJR 1.293 SNIP 2.127
A Consistent Methodology Based Parameter Estimation for a Lactic Acid Bacteria Fermentation Model

Lactic acid bacteria are used in many industrial applications, e.g. as starter cultures in the dairy industry or as probiotics, and research on their cell production is highly required. A first principles kinetic model was developed to describe and understand the biological, physical, and chemical mechanisms in a lactic acid bacteria fermentation. We present here a consistent approach for a methodology based parameter estimation for a lactic acid fermentation. In the beginning, just an initial knowledge based guess of parameters was available and an initial parameter estimation of the complete set of parameters was performed in order to get a good model fit to the data. However, not all parameters are identifiable with the given data set and model structure. Sensitivity, identifiability, and uncertainty analysis were completed and a relevant identifiable subset of parameters was determined for a new parameter estimation including an evaluation of the correlation and confidence intervals of those parameters to double-check identifiability issues. Such a consistent approach supports process modelling and understanding as i.e., one avoids questionable interpretations caused by estimates of actually unidentifiable parameters.
Activity of type I methanotrophs dominates under high methane concentration: Methanotrophic activity in slurry surface crusts as influenced by methane, oxygen, and inorganic nitrogen

Livestock slurry is a major source of atmospheric methane (CH\textsubscript{4}), but surface crusts harboring methane-oxidizing bacteria (MOB) could mediate against CH\textsubscript{4} emissions. This study examined conditions for CH\textsubscript{4} oxidation by in situ measurements of oxygen (O\textsubscript{2}) and nitrous oxide (N\textsubscript{2}O), as a proxy for inorganic N transformations, in intact crusts using microsensors. This was combined with laboratory incubations of crust material to investigate the effects of O\textsubscript{2}, CH\textsubscript{4}, and inorganic N on CH\textsubscript{4} oxidation, using \textsuperscript{13}CH\textsubscript{4} to trace C incorporation into lipids of MOB. Oxygen penetration into the crust was 2 to 14 mm, confining the potential for aerobic CH\textsubscript{4} oxidation to a shallow layer. Nitrous oxide accumulated within or below the zone of O\textsubscript{2} depletion. With 102 ppmv CH\textsubscript{4} there was no O\textsubscript{2} limitation on CH\textsubscript{4} oxidation at O\textsubscript{2} concentrations as low as 2%, whereas CH\textsubscript{4} oxidation at 104 ppmv CH\textsubscript{4} was reduced at \textless 5% O\textsubscript{2}. As hypothesized, CH\textsubscript{4} oxidation was in general inhibited by inorganic N, especially NO\textsubscript{2} -, and there was an interaction between N inhibition and O\textsubscript{2} limitation at 102 ppmv CH\textsubscript{4}, as indicated by consistently stronger inhibition of CH\textsubscript{4} oxidation by NH\textsubscript{4} + and NO\textsubscript{3} - at 3% compared with 20% O\textsubscript{2}. Recovery of \textsuperscript{13}C in phospholipid fatty acids suggested that both Type I and Type II MOB were active, with Type I dominating high-concentration CH\textsubscript{4} oxidation. Given the structural heterogeneity of crusts, CH\textsubscript{4} oxidation activity likely varies spatially as constrained by the combined effects of CH\textsubscript{4}, O\textsubscript{2}, and inorganic N availability in microsites.

General information
State: Published
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Scopus rating (2014): SJR 1.274 SNIP 1.271 CiteScore 2.66
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Scopus rating (2013): SJR 1.318 SNIP 1.275 CiteScore 2.7
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.371 SNIP 1.22 CiteScore 2.51
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.47 SNIP 1.359 CiteScore 2.53
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.299 SNIP 1.314
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Scopus rating (2009): SJR 1.425 SNIP 1.354
Adding Value to Bioethanol through a Purification Process Revamp

A comprehensive technical feasibility study was conducted of a bioethanol demonstration plant with the aim of converting parts of an existing fuel-grade bioethanol production into a more valuable solvent-grade ethanol. The study focuses on the separation unit, which consists of three consecutive distillation columns and a dehydration step using molecular sieves. This separation unit did not permit sufficient removal of crotonaldehyde and methanol for obtaining solvent-grade ethanol. Therefore, an additional distillation column after the dehydration step was investigated by simulation. It is operated at subatmospheric pressure and enables simultaneous removal of methanol, crotonaldehyde, and water in the distillate. The distillate meets the fuel-grade ethanol specifications, while the bottom product meets the solvent-grade specifications. It enables around 70% solvent-grade ethanol production and employs a vacuum pump that is already used in the considered plant. A stationary operating point is characterized by online operational data and experimental results of liquid samples. Particular emphasis during the characterization is put on trace compounds. Ethanol and the following 13 trace compounds were analyzed experimentally: Acetaldehyde, 1-propanal, 1-butanal, crotonaldehyde, benzaldehyde, ethyl acetate, methanol, 1-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-1-butanol, and 3-methyl-1-butanol. A simulation platform was established and evaluated with excellent agreement compared to the operational data. The beer composition (separation unit feed) and a complete stream summary for the separation unit is provided.
Adiabatic continuous stirred tank reactor
The present report documents the adiabatic CSTR experimental setup after it was refurbished in September 2017. The goal of the refurbishment was firstly to enable computer control of the experiment using the Open Process Control Unified Architecture (OPC-UA) standard, and secondly to improve the experiment for use in course 28845 Chemical Reaction Engineering Laboratory.
Initially the experimental setup is described in terms of programmable logic controller (PLC) hardware, laboratory apparatus and software. This is followed by a description of how to connect to the PLC via OPC-UA.
The appendix contains an experimental guide for use in course 28845, step-by-step instructions on how to control the setup with a computer, sample code and datasheets.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering
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Advanced fabrication of porous ceramic multilayers for membrane applications

Affinity Electrophoresis for Analysis of Catalytic Module-Carbohydrate Interactions
Affinity electrophoresis has long been used to study the interaction between proteins and large soluble ligands. The technique has been found to have great utility for the examination of polysaccharide binding by proteins, particularly carbohydrate binding modules (CBMs). In recent years, carbohydrate surface binding sites of proteins mostly enzymes have also been investigated by this method. Here, we describe a protocol for identifying binding interactions between enzyme catalytic modules and a variety of carbohydrate ligands.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering
Authors: Schroll-Fleischer, E. (Intern), Wu, H. (Intern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
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Advanced fabrication of porous ceramic multilayers for membrane applications

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Affinity Electrophoresis for Analysis of Catalytic Module-Carbohydrate Interactions
Affinity electrophoresis has long been used to study the interaction between proteins and large soluble ligands. The technique has been found to have great utility for the examination of polysaccharide binding by proteins, particularly carbohydrate binding modules (CBMs). In recent years, carbohydrate surface binding sites of proteins mostly enzymes have also been investigated by this method. Here, we describe a protocol for identifying binding interactions between enzyme catalytic modules and a variety of carbohydrate ligands.

General information
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A generic methodology for processing route synthesis and design based on superstructure optimization

In this paper, a systematic framework for novel and sustainable synthesis-design of processing routes is presented along with the associated computer-aided methods and tools. In Stage 1, superstructure optimization is used to determine the optimal processing route(s). In Stage 2, the design issues are resolved and targets for improvement are identified through the use of integrated tools. In Stage 3, new alternatives are generated using the selected route and the previously identified targets. In addition to the various computer-aided tools, two special tools are presented: (1) a database employing a specially developed knowledge representation system, and (2) Super-O, a software interface that guides users through the formulation and solution of synthesis problems. Super-O transfers data between the different tools, including a library of generic models, representing a wide range of processing options. Application of the synthesis and design stages is highlighted through two case studies (biorefinery and carbon capture-utilization).

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CAPEC-PROCESS, Technical University of Denmark
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- Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
A grid-independent EMMS/bubbling drag model for bubbling and turbulent fluidization

The EMMS/bubbling drag model takes the effects of meso-scale structures (i.e. bubbles) into modeling of drag coefficient and thus improves coarse-grid simulation of bubbling and turbulent fluidized beds. However, its dependence on grid size has not been fully investigated. In this article, we adopt a two-step scheme to extend the EMMS/bubbling model to the sub-grid level. Thus the heterogeneity index, HD, which accounts for the hydrodynamic disparity between homogeneous and heterogeneous fluidization, can be correlated as a function of both local voidage and slip velocity. Simulations over a periodic domain show the new drag model is less sensitive to grid size because of the additional dependence on local slip velocity. When applying the new drag model to simulations of realistic bubbling and turbulent fluidized beds, we find grid-independent results are easier to obtain for high-velocity turbulent fluidized bed cases. The simulation results indicate that the extended EMMS/bubbling drag model is a potential method for coarse-grid simulations of large-scale fluidized beds.
A model library for simulation and benchmarking of integrated urban wastewater systems

This paper presents a freely distributed, open-source toolbox to predict the behaviour of urban wastewater systems (UWS). The proposed library is used to develop a system-wide Benchmark Simulation Model (BSM-UWS) for evaluating (local/global) control strategies in urban wastewater systems (UWS). The set of models describe the dynamics of flow rates and major pollutants (COD, TSS, N and P) within the catchment (CT), sewer network (SN), wastewater treatment
plant (WWTP) and river water system (RW) for a hypothetical, though realistic, UWS. Evaluation criteria are developed to allow for direct assessment of the river water quality instead of the traditional emission based metrics (for sewer overflows and WWTP discharge). Three case studies are included to illustrate the applicability of the proposed toolbox and also demonstrate the potential benefits of implementing integrated control in the BSM-UWS platform. Simulation results show that the integrated control strategy developed to maximize the utilization of the WWTP's capacity represents a balanced choice in comparison to other options. It also improves the river water quality criteria for unionized ammonia and dissolved oxygen by 62% and 6%, respectively.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University, Aquafin NV
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Scopus rating (2016): CiteScore 4.8 SJR 1.936 SNIP 2.112
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.119 SNIP 2.172 CiteScore 4.67
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.065 SNIP 2.483 CiteScore 5.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.082 SNIP 2.458 CiteScore 4.8
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.829 SNIP 2.012 CiteScore 3.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.68 SNIP 2.096 CiteScore 3.52
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.684 SNIP 2.221
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.33 SNIP 1.965
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.131 SNIP 1.892
Scopus rating (2007): SJR 1.125 SNIP 1.907
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.962 SNIP 1.743
Scopus rating (2005): SJR 0.927 SNIP 1.595
Analysis and Modelling of an Industrial Pressure Filtration using Process Data

In order to understand a series of pressure leaf filters located in the downstream line of a bio-based production site, historical process data have been analysed. In general, changing raw materials induce variability into the pressure profiles and thereby cycle durations of the manually reinitialised dead-end filtrations. The absence of a true steady state results in uncertainty about the optimal way of running the filters, and staff members alter the operational specifications frequently. It appears that, in some cases, this propagates disturbances rather than ameliorate them. Statistical analyses are carried out to illustrate the current situation and especially allow quantifying the extent of the uncertainties. Furthermore, significant correlations between process variables are revealed and economically motivated operational objectives are identified. Secondly, working towards on-line predictions of filtration performance, a model is presented. It is based on classical filtration theory and requires only commonly available measurements (pressure, flow, viscosity). The generated predictions are found to be acceptable for many cycles, but in some cases fail due to non-modelled effects, motivating further work.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, CP Kelco ApS
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Analyzing Activities of Lytic Polysaccharide Monooxygenases by Liquid Chromatography and Mass Spectrometry

Lytic polysaccharide monooxygenases perform oxidative cleavage of glycosidic bonds in various polysaccharides. The majority of LMPOs studied so far possess activity on either cellulose or chitin and analysis of these activities is therefore the main focus of this review. Notably, however, the number of LPMOs that are active on other polysaccharides is increasing. The products generated by LPMOs from cellulose are either oxidized in the downstream end (at C1) or upstream end (at C4), or at both ends. These modifications only result in small structural changes, which makes both chromatographic separation and product identification by mass spectrometry challenging. The changes in physicochemical properties that are associated with oxidation need to be considered when choosing analytical approaches. C1 oxidation leads to a sugar that is no longer reducing but instead has an acidic functionality, whereas C4 oxidation leads to products that are inherently labile at high and low pH and that exist in a keto-gemdiol equilibrium that is strongly shifted toward the gemdiolin aqueous solutions. Partial degradation of C4-oxidized products leads to the formation of native products which could explain why some authors claim to have observed glycoside hydrolase activity for LPMOs. Notably, apparent glycoside hydrolase activity may also be due to small amounts of contaminating glycoside hydrolases since these normally have much higher catalytic rates than LPMOs. The low catalytic turnover rates of LPMOs necessitate the use of sensitive product detection methods, which limits the analytical possibilities considerably. Modern liquid chromatography and mass spectrometry have become essential tools for evaluating LPMO activity, and this chapter provides an overview of available methods together with a few novel tools. The methods described constitute a suite of techniques for analyzing oxidized carbohydrate products, which can be applied to LPMOs as well as other carbohydrate-active redox enzymes.
model building procedure and process characterization.

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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre
Authors: Tajsoleiman, T. (Intern), Semenova, D. (Intern), Oliveira Fernandes, A. C. (Intern), Huusom, J. K. (Intern), Gernaey, K. V. (Intern), Krühne, U. (Intern)
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**An Empirical Model for Carbon Recovery in a Rotating Belt Filter and Its Application in the Frame of Plantwide Evaluation**
The rotating belt filter (RBF) is an emerging and enabling technology for carbon recovery and also an alternative to the primary clarifier (PC), sludge thickening and dewatering. A recent study indicates that the RBF has the potential to reduce capital cost, footprint and improve energy and nutrient recovery in comparison to a conventional PC. Moreover, it is also believed that the RBF can fractionate carbon (enrichment of cellulose, namely toilet paper) based on particulate size, more efficiently than a PC. It is, therefore, necessary to understand and quantify the uniqueness of the RBF performance to maximize plant-wide benefits when retrofitted in existing wastewater treatment plants (WWTPs). Thus, a rigorous plant-wide study is required to interpret the deeper influence of an RBF on the major downstream units (such as activated sludge tanks, sludge digester, etc.). This study emphasizes the development of a simplified empirical model for describing carbon recovery in an RBF and the impact of the RBF implementation on plant-wide evaluation.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Trojan Technologies
Authors: Behera, C. R. (Intern), Daynouri-Pancino, F. (Ekstern), Santoro, D. (Ekstern), Gernaey, K. (Intern), Sin, G. (Intern)
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**A New Functional Classification of Glucuronoyl Esterases by Peptide Pattern Recognition**
Glucuronoyl esterases are a novel type of enzymes believed to catalyze the hydrolysis of ester linkages between lignin and glucuronoxylan in lignocellulosic biomass, linkages known as lignin carbohydrate complexes. These complexes contribute to the recalcitrance of lignocellulose. Glucuronoyl esterases are a part of the microbial machinery for
lignocellulose degradation and coupling their role to the occurrence of lignin carbohydrate complexes in biomass is a desired research goal. Glucuronoyl esterases have been assigned to CAZymes family 15 of carbohydrate esterases, but only few examples of characterized enzymes exist and the exact activity is still uncertain. Here peptide pattern recognition is used as a bioinformatic tool to identify and group new CE15 proteins that are likely to have glucuronoyl esterase activity. 1024 CE15-like sequences were drawn from GenBank and grouped into 24 groups. Phylogenetic analysis of these groups made it possible to pinpoint groups of putative fungal and bacterial glucuronoyl esterases and their sequence variation. Moreover, a number of groups included previously undescribed CE15-like sequences that are distinct from the glucuronoyl esterases and may possibly have different esterase activity. Hence, the CE15 family is likely to comprise other enzyme functions than glucuronoyl esterase alone. Gene annotation in a variety of fungal and bacterial microorganisms showed that coprophilic fungi are rich and diverse sources of CE15 proteins. Combined with the lifestyle and habitat of coprophilic fungi, they are predicted to be excellent candidates for finding new glucuronoyl esterase genes.

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A novel back-up control structure to manage nonroutine steam upsets in industrial methanol distillation columns

Industrial methanol production plants have extensive heat integration to achieve energy efficient operations where steam generated from these heat integration operations are used to provide reboiler duty for methanol distillation columns that purify crude methanol produced into industrial AA grade methanol at a relatively high rate of product recovery. As such, fluctuation in steam supply due to non-routine process changes can lead to result in off specification distillation operations which results insignificant economic losses. This work has investigated and identified the causes and consequences of these steam flow disturbances and developed two backup control structures to operate the distillation columns within specification during steam flow disturbances. One of the new control structures is based on model predictive control (MPC), while the other is a PID-based control structure with a novel supervisory layer to control the column during these non-routine process upsets. These control schemes were tested against realistic reboiler duty disturbances that can occur in an industrial process. The tests revealed that both the MPC and supervisory systems control structures are able to regulate the process, even during sudden drops in reboiler duty. However, the cost of implementation and the relative simplicity will likely favour the implementation of the supervisory control structure in an industrial environment.

A novel fuzzy-logic control strategy minimizing N2O emissions

A novel control strategy for achieving low N2O emissions and low effluent NH4+ concentration is here proposed. The control strategy uses the measurements of ammonium and nitrate concentrations in inlet and outlet of the aerobic zone of a wastewater treatment plant to calculate a ratio indicating the balance among the microbial groups. More specifically, the ratio will indicate if there is a complete nitrification. In case nitrification is not complete, the controller will adjust the aeration level of the plant in order to inhibit the production of N2O from AOB and HB denitrification. The controller was implemented using the fuzzy logic approach. It was comprehensively tested for different model structures and different sets of model parameters with regards to its ability of mitigating N2O emissions for future applications in real wastewater treatment plants. It is concluded that the control strategy is useful for those plants having AOB denitrification as the main N2O producing process. However, in treatment plants having incomplete NH2OH oxidation as the main N2O producing pathway, a cascade controller configuration adapting the oxygen supply to respect only the effluent ammonium concentration limits was found to be more effective to ensure low N2O emissions.
A novel in situ measurement method of bubble sizes in bioreactors using a high speed camera

Mass transfer of oxygen from the gas phase to the liquid phase is the rate limiting phenomenon in many industrial aerobic fermentation processes. This phenomenon is often described by the rate constant $k_La$, which remains a key performance indicator for scale up and general operation of fermentation processes. The attributing variables to the rate constant, the mass transfer resistance $k_L$ and interfacial surface area $a$, are however very rarely individually identifiable from standard experimental analysis. This co-dependency of the variables on the rate constant limits the understanding of how process conditions affect the mass transfer rate, and hence a tool for identifying them individually is required. Available correlations for these variables are predominantly system dependent and therefore not necessarily valid in the process of interest. Currently available measurement techniques to identify bubble size require knowledge or assumptions regarding the gas flow direction to deduce the bubble size.

An optical method for determining the interfacial surface area, based on bubble size identification has been developed using a high speed camera and an endoscope. This novel method has been applied to bioreactors at different conditions in terms of power input, gas flow rate and viscosity. This in situ measurement illustrates the effect of process conditions on the size of the bubbles. The information on bubble sizes at different conditions is a valuable input to mechanistic models regarding gas-liquid mass transfer, for example computational fluid dynamics (CFD) models, in which the bubble size is a key input parameter.

A Novel Method for Detecting and Computing Univolatility Curves in Ternary Mixtures

Residue curve maps (RCMs) and univolatility curves are crucial tools for analysis and design of distillation processes. Even in the case of ternary mixtures, the topology of these maps is highly non-trivial. We propose a novel method allowing detection and computation of univolatility curves in homogeneous ternary mixtures independently of the presence of azeotropes, which is particularly important in the case of zeotropic mixtures. The method is based on the analysis of the geometry of the boiling temperature surface constrained by the univolatility condition. The introduced concepts of the generalized univolatility and unidistribution curves in the three dimensional composition – temperature state space lead to a simple and efficient algorithm of computation of the univolatility curves. Two peculiar ternary systems, namely diethylamine – chloroform – methanol and hexane – benzene – hexafluorobenzene are used for illustration. When varying pressure, tangential azeotropy, bi-ternary azeotropy, saddle-node ternary azeotrope, and bi-binary azeotropy are identified. Moreover, rare univolatility curves starting and ending on the same binary side are found. In both examples, a distinctive crossing shape of the univolatility curve appears as a consequence of the existence of a common tangent point between the three dimensional univolatility hypersurface and the boiling temperature surface.
A novel model-based control strategy for aerobic filamentous fungal fed-batch fermentation processes

A novel model-based control strategy has been developed for filamentous fungal fed-batch fermentation processes. The system of interest is a pilot scale (550L) filamentous fungus process operating at Novozymes A/S. In such processes, it is desirable to maximize the total product achieved in a batch in a defined process time. In order to achieve this goal, it is important to maximize both the product concentration, and also the total final mass in the fed-batch system. To this end, we describe the development of a control strategy which aims to achieve maximum tank fill, while avoiding oxygen limited conditions. This requires a two stage approach: (i) calculation of the tank start fill; and (ii) on-line control in order to maximize fill subject to oxygen transfer limitations. First, a mechanistic model was applied off-line in order to determine the appropriate start fill for processes with four different sets of process operating conditions for the stirrer speed, headspace pressure, and aeration rate. The start fills were tested with eight pilot scale experiments using a reference process operation. An on-line control strategy was then developed, utilizing the mechanistic model which is recursively updated using on-line measurements. The model was applied in order to predict the current system states, including the biomass concentration, and to simulate the expected future trajectory of the system until a specified end time. In this way, the desired feed rate is updated along the progress of the batch taking into account the oxygen mass transfer conditions and the expected future trajectory of the mass. The final results show that the target fill was achieved to within 5% under the maximum fill when tested using eight pilot scale batches, and over filling was avoided. The results were reproducible, unlike the reference experiments which show over 10% variation in the final tank fill, and this also includes over filling. The variance of the final tank fill is reduced by over 74%, meaning that it is possible to target the final maximum fill reproducibly. The product concentration achieved at a given set of process conditions was unaffected by the control strategy. Biotechnol. Bioeng. 2017;9999: 1–10. © 2017 Wiley Periodicals, Inc.
Application of a computer-aided framework for the design of CO2 capture and utilization processes

Carbon dioxide capture and utilization is a vital element of carbon dioxide emission reduction to address global warming. An integrated, computer-aided framework has been developed to achieve this. This framework adopts a three-stage approach to sustainable process synthesis-design: (i) process synthesis, (ii) process design and (iii) innovative design. In the first stage, reaction path synthesis is used to determine the reactions and products that are considered in processing route selection and/or generation. Various scenarios are then considered for the superstructure optimization. The selected processing route(s) is then designed and analyzed in Stage 2 to determine “hot spots” and the targets for improvement. Finally, these targets are improved in Stage 3 through the use of process integration and process intensification methods. In this work, over 150 reactions are considered for 1-3 reaction steps. Then, the superstructure optimization is performed on a network containing 13 likely products giving 30 feasible processing routes, considering different scenarios and objectives. Stages 2 and 3 have been applied to the optimal solution of the first scenario, which selects the production of dimethyl carbonate via ethylene carbonate; in Stage 3, the downstream separation is targeted for improvement and the use of reactive distillation as the more sustainable alternative, is obtained.
Application of a computer-aided framework for the design of CO₂ capture and utilization processes

Currently, close to 50 gigatonnes per year of carbon dioxide are emitted to the atmosphere. As carbon dioxide is the dominant greenhouse gas that contributes to sustainability concerns, these emissions need to be targeted for reduction. Carbon dioxide capture and utilization shows promise due to the ability to offset (economically) the cost of carbon capture. However, in order to ensure the sustainability of these processes, methods and tools need to be developed and implemented. To this end, a framework for sustainable process synthesis-design, comprising three stages, (1) synthesis, (2) design, and (3) innovation, has been developed. In order to facilitate the implementation and ensure sustainability, this framework integrates a number of computer-aided methods and tools, that are important for carbon dioxide capture and utilization. Applying this framework helps to address the questions about carbon dioxide capture, storage and utilization on several scales (local as well as global). For example, which higher value chemicals can be produced, what are their current demands, and how much of the carbon dioxide would be utilized?

This framework has been applied to the design and analysis of carbon dioxide capture and utilization processes from coal-fired power plant flue gas to produce various value-added chemical products, including methanol, dimethyl carbonate, dimethyl ether, succinic acid and acetic acid, via conversion. First, the processing route is selected from a network of alternatives. This stage incorporates reaction path synthesis to find different reaction opportunities (currently over 100 reactions have been generated producing commercial chemical products), a database to store the information, and an interface, Super-O, to facilitate the synthesis. In this way, unique opportunities and products are explored. Second, the selected processing route is designed and analyzed by using simulation software and sustainability (economic, environmental and LCA) analysis tools. From this stage, hot spots and areas for improvement are also generated. Third, the targets for improvement are used to develop novel and more sustainable design alternatives, including the use of process intensification. As a result, it is possible to identify non-trade-off carbon dioxide capture and conversion processes. The production of methanol and dimethyl carbonate have been designed and analyzed to show that conversion processes can be economically competitive and environmentally beneficial (carbon dioxide reducing). This work will present the application of reaction path synthesis combined with superstructure optimization and an appropriate database, to propose sustainable processing routes, with negative net CO₂ emissions, for a class of valuable chemicals.
Application of a Crossover Equation of State to Describe Phase Equilibrium and Critical Properties of n-Alkanes and Methane/n-Alkane Mixtures

Crossover equations of state (EOSs) are models that incorporate density fluctuations into mean-field thermodynamic models, changing their behavior close to the critical point. In this way, they are capable of describing the analytical behavior of fluids far from the critical region and the asymptotic one near the critical point. Although several crossover EOSs have been developed in the last decades their use in modeling industrial processes is rather limited. In this work, we use the crossover Soave–Redlich–Kwong (CSRK) to describe phase equilibrium and critical properties of pure n-alkanes and methane/n-alkane binary mixtures and compare the results to two other modeling approaches of the SRK EOS. In the case of the pure fluids, CSRK gives an accurate overall description of the phase equilibrium and critical properties; nevertheless, a minor increase in the deviation of the saturation pressure and other properties is observed when compared to that of the mean-field model. For the binary mixtures, an improvement in the description of the critical volumes is seen, while, for the other properties, similar results are obtained.

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A mechanistic model-based soft sensor is developed and validated for 550L filamentous fungus fermentations operated at Novozymes A/S. The soft sensor is comprised of a parameter estimation block based on a stoichiometric balance, coupled to a dynamic process model. The on-line parameter estimation block models the changing rates of formation of product, biomass, and water, and the rate of consumption of feed using standard, available on-line measurements. This parameter estimation block, is coupled to a mechanistic process model, which solves the current states of biomass, product, substrate, dissolved oxygen and mass, as well as other process parameters including kLa, viscosity and partial pressure of CO2. State estimation at this scale requires a robust mass model including evaporation, which is a factor not often considered at smaller scales of operation. The model is developed using a historical dataset of eleven batches from the fermentation pilot plant (550L) at Novozymes A/S. The model is then implemented on-line in 550L fermentation processes operated at Novozymes A/S in order to validate the state estimator model on fourteen new batches utilizing a new strain. The product concentration in the validation batches was predicted with an average root mean sum of squared error (RMSSE) of 16.6%. In addition, calculation of the Janus coefficient for the validation batches shows a suitably calibrated model. The robustness of the model prediction is assessed with respect to the accuracy of the input data. Parameter estimation uncertainty is also carried out. The application of this on-line state estimator allows for on-line monitoring of pilot scale batches, including real-time estimates of multiple parameters which are not able to be monitored on-line. With successful application of a soft sensor at this scale, this allows for improved process monitoring, as well as opening up further possibilities for on-line control algorithms, utilizing these on-line model outputs. This article is protected by copyright. All rights reserved
Application of Iterative Robust Model-based Optimal Experimental Design for the Calibration of Biocatalytic Models

The aim of model calibration is to estimate unique parameter values from available experimental data, here applied to a biocatalytic process. The traditional approach of first gathering data followed by performing a model calibration is inefficient, since the information gathered during experimentation is not actively used to optimise the experimental design. By applying an iterative robust model-based optimal experimental design, the limited amount of data collected is used to design additional informative experiments. The algorithm is used here to calibrate the initial reaction rate of an ω-transaminase catalysed reaction in a more accurate way. The parameter confidence region estimated from the Fisher Information Matrix is compared with the likelihood confidence region, which is a more accurate, but also a computationally more expensive method. As a result, an important deviation between both approaches is found, confirming that linearisation methods should be applied with care for nonlinear models. This article is protected by copyright. All rights reserved.

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A Reaction Database for Small Molecule Pharmaceutical Processes Integrated with Process Information

This article describes the development of a reaction database with the objective to collect data for multiphase reactions involved in small molecule pharmaceutical processes with a search engine to retrieve necessary data in investigations of reaction-separation schemes, such as the role of organic solvents in reaction performance improvement. The focus of this reaction database is to provide a data rich environment with process information available to assist during the early stage synthesis of pharmaceutical products. The database is structured in terms of reaction classification of reaction types; compounds participating in the reaction; use of organic solvents and their function; information for single step and multistep reactions; target products; reaction conditions and reaction data. Information for reactor scale-up together with information for the separation and other relevant information for each reaction and reference are also available in the database. Additionally, the retrieved information obtained from the database can be evaluated in terms of sustainability using well-known “green” metrics published in the scientific literature. The application of the database is illustrated through the synthesis of ibuprofen, for which data on different reaction pathways have been retrieved from the database and compared using “green” chemistry metrics.

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A review of control strategies for manipulating the feed rate in fed-batch fermentation processes

A majority of industrial fermentation processes are operated in fed-batch mode. In this case, the rate of feed addition to the system is a focus for optimising the process operation, as it directly impacts metabolic activity, as well as directly affecting the volume dynamics in the system. This review covers a range of strategies which have been employed to use the feed rate as a manipulated variable in a control strategy. The feed rate is chosen as the focus for this review, as it is seen that this variable may be used towards many different objectives depending on the process of interest, the characteristics of the strain, or the product being produced, which leads to different drivers for process optimisation. This review summarises the methods, as well as focusing on the different objectives for the controllers, and the choice of measured variables involved in the strategy. The discussion includes a summary of considerations for control strategy development.
A simplified kinetic and mass transfer modelling of the thermal hydrolysis of vegetable oils

This work presents a combined modelling approach to investigate the kinetics and mass transfer effects on the hydrolysis of vegetable oils under subcritical conditions. The primary purpose of this simplified model is to interpret experimental data collected from typical batch tests and to estimate parameters for the proposed model. Due to its heterogeneous nature, the hydrolysis reaction is affected not only by the chemical kinetics but also by the rate of mass transfer between the oil and water as well as their specific contact area in this two phase emulsion. Considering these properties, a model was developed and evaluated by comparing the results with experimental data from literature. The model included among others the mass transfer coefficient as a function of operation and process variables, e.g. agitation speed, temperature, pressure, density and viscosity. Thereafter, uncertainty analysis was performed to assess the accuracy of estimated parameters and model predictions. The parameter estimation results showed that while the parameter estimates were accurate, however the pairwise correlation between estimates were significant. This indicates that the available experimental data is not fit to uniquely identify the mass and kinetic parameters requiring further and better design optimal experiment. The uncertainty analysis showed that model prediction uncertainty due to parameter estimation errors were rather negligible. Therefore it is recommended that the model be used for process analysis and improvement accompanied by Monte Carlo uncertainty analysis. Since the lack of experimental data is a crucial issue in the hydrolysis
of vegetable oils, this model-based analysis of data is of substantial value to provide necessary information for detailed modeling and characterization of the process.

Aspergillus hancockii sp. Nov., a biosynthetically talented fungus endemic to southeastern Australian soils

Aspergillus hancockii sp. nov., classified in Aspergillus subgenus Circumdati section Flavi, was originally isolated from soil in peanut fields near Kumbia, in the South Burnett region of southeast Queensland, Australia, and has since been found occasionally from other substrates and locations in southeast Australia. It is phylogenetically and phenotypically related most closely to A. leporis States and M. Chr., but differs in conidial colour, other minor features and particularly in metabolite profile. When cultivated on rice as an optimal substrate, A. hancockii produced an extensive array of 69 secondary metabolites. Eleven of the 15 most abundant secondary metabolites, constituting 90% of the total area under the curve of the HPLC trace of the crude extract, were novel. The genome of A. hancockii, approximately 40 Mbp, was sequenced and mined for genes encoding carbohydrate degrading enzymes identified the presence of more than 370 genes in 114 gene clusters, demonstrating that A. hancockii has the capacity to degrade cellulose, hemicellulose, lignin, pectin, starch, chitin, cutin and fructan as nutrient sources. Like most Aspergillus species, A. hancockii exhibited a diverse secondary metabolite gene profile, encoding 26 polyketide synthase, 16 nonribosomal peptide synthase and 15 nonribosomal peptide synthase-like enzymes.
In this work, a systematic identification method for thermodynamic property modelling is proposed. The aim of the method is to improve the quality of phase equilibria prediction by group contribution based property prediction models. The method is applied to lipid systems where the Original UNIFAC model is used. Using the proposed method for estimating the interaction parameters using only VLE data, a better phase equilibria prediction for both VLE and SLE was obtained. The results were validated and compared with the original model performance.
A systematic model identification method for chemical transformation pathways – the case of heroin biomarkers in wastewater

This study presents a novel statistical approach for identifying sequenced chemical transformation pathways in combination with reaction kinetics models. The proposed method relies on sound uncertainty propagation by considering parameter ranges and associated probability distribution obtained at any given transformation pathway levels as priors for parameter estimation at any subsequent transformation levels. The method was applied to calibrate a model predicting the transformation in untreated wastewater of six biomarkers, excreted following human metabolism of heroin and codeine. The method developed was compared to parameter estimation methods commonly encountered in literature (i.e., estimation of all parameters at the same time and parameter estimation with fix values for upstream parameters) by assessing the model prediction accuracy, parameter identifiability and uncertainty analysis. Results obtained suggest that the method developed has the potential to outperform conventional approaches in terms of prediction accuracy, transformation pathway identification and parameter identifiability. This method can be used in conjunction with optimal experimental designs to effectively identify model structures and parameters. This method can also offer a platform to promote a closer interaction between analytical chemists and modellers to identify models for biochemical transformation pathways, being a prominent example for the emerging field of wastewater-based epidemiology.
Automated Determination of Oxygen-Dependent Enzyme Kinetics in a Tube-in-Tube Flow Reactor

Enzyme-mediated oxidation is of particular interest to synthetic organic chemists. However, the implementation of such systems demands knowledge of enzyme kinetics. Conventionally collecting kinetic data for biocatalytic oxidations is fraught with difficulties such as low oxygen solubility in water and limited oxygen supply. Here, we present a novel method for the collection of such kinetic data using a pressurized tube-in-tube reactor, operated in the low-dispersed flow regime to generate time-series data, with minimal material consumption. Experimental development and validation of the instrument revealed not only the high degree of accuracy of the kinetic data obtained, but also the necessity of making measurements in this way to enable the accurate evaluation of high $K_{MO}$ enzyme systems. For the first time, this paves the way to integrate kinetic data into the protein engineering cycle.

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Beamstop-based low-background ptychography to image weakly scattering objects

In recent years, X-ray ptychography has been established as a valuable tool for high-resolution imaging. Nevertheless, the spatial resolution and sensitivity in coherent diffraction imaging are limited by the signal that is detected over noise and over background scattering. Especially, coherent imaging of weakly scattering specimens suffers from incoherent background that is generated by the interaction of the central beam with matter along its propagation path in particular close to and inside of the detector. Common countermeasures entail evacuated flight tubes or detector-side beamstops, which improve the experimental setup in terms of background reduction or better coverage of high dynamic range in the diffraction patterns. Here, we discuss an alternative approach: we combine two ptychographic scans with and without beamstop and reconstruct them simultaneously taking advantage of the complementary information contained in the two scans. We experimentally demonstrate the potential of this scheme for hard X-ray ptychography by imaging a weakly scattering object composed of catalytic nanoparticles and provide the analysis of the signal-to-background ratio in the diffraction patterns.

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Biocatalysis

Biocatalysis is important for addressing global challenges: climate change, substitution of fossils, feeding a growing population—basically because bioprocessing in food, feed, and nonfood industries improves resource efficiency, getting more out of the raw biomaterials. Microbial enzymes are the active elements in biocatalysis. Enzymes are specific and efficient (not used up, but reusable). The small enzyme molecules contribute significantly to making industrial processes more sustainable, by changing from chemical processes to enzymatic (biocatalytic) processes, being milder, using less energy, producing less waste water. Enzymes and biocatalysis are key elements in sustainable production of biobased products in the new bioeconomy era.

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, University of Delhi
Biodiversity and species competition regulate the resilience of microbial biofilm community

The relationship between biodiversity and ecosystem stability is poorly understood in microbial communities. Biofilm communities in small bioreactors called microbial electrolysis cells (MEC) contain moderate species numbers and easy tractable functional traits, thus providing an ideal platform for verifying ecological theories in microbial ecosystems. Here, we investigated the resilience of biofilm communities with a gradient of diversity, and explored the relationship between biodiversity and stability in response to a pH shock. The results showed that all bioreactors could recover to stable performance after pH disturbance, exhibiting a great resilience ability. A further analysis of microbial composition showed that the rebound of Geobacter and other exoelectrogens contributed to the resilient effectiveness, and that the presence of Methanobrevibacter might delay the functional recovery of biofilms. The microbial communities with higher diversity tended to be recovered faster, implying biofilms with high biodiversity showed better resilience in response to environmental disturbance. Network analysis revealed that the negative interactions between the two dominant genera of Geobacter and Methanobrevibacter increased when the recovery time became longer, implying the internal resource or spatial competition of key functional taxa might fundamentally impact the resilience performances of biofilm communities. This study provides new insights into our understanding of the relationship between diversity and ecosystem functioning.
Biomass ignition in mills and storages – is it explained by conventional thermal ignition theory?

Self-ignition temperatures determined in the framework of conventional thermal ignition theory does not explain why biomass is much more susceptible to spontaneous ignition in power plant mills or storages. Examining the onset of reactions at low temperatures may provide a better understanding of the process, which can then be incorporated into refined models of self-ignition for biomass and other organic solids. In the present study, the slow, transient heating of several lignocellulosic biomasses and a bituminous coal from ambient temperature to around 300° C were investigated in a lab scale tube oven, with sample sizes between 11–40 g. Tests were carried out under oxidizing (20 % O2) and inert atmospheres. Judged by off-gas measurements of CO and CO2, a reaction onset could be seen at temperatures below 100° C. Under oxidizing atmosphere, reactions were more intense and set off earlier, suggesting that a heterogeneous
oxidation is the dominating mechanism in self-ignition. It could also be shown that both mechanisms compete for reactive material. While oxidation was exothermic, pyrolysis was largely thermally neutral in these experiments. Reaction behavior was seen to depend highly on the material, and the results indicate that higher ash contents may promote reaction onset. However, further work is needed to arrive at a comprehensive model of self-ignition.

**Bioprocess intensification for the effective production of chemical products**

The further implementation of new bioprocesses, using biocatalysts in various formats, for the synthesis of chemicals is highly dependent upon effective process intensification. The need for process intensification reflects the fact that the conditions under which a biocatalyst carries out a reaction in nature are far from those which are optimal for industrial processes. In this paper the rationale for intensification will be discussed, as well as the four complementary approaches used today to achieve bioprocess intensification. Two of these four approaches are based on alteration of the biocatalyst (either by protein engineering or metabolic engineering), resulting in an extra degree of freedom in the process design. To date, biocatalyst engineering has been developed independently from the conventional process engineering methodology to intensification. Although the integration of these two methodologies has now started, in the future synergistic integration should enable many new opportunities for bioprocesses for the production of chemicals.
Biorefinery Sustainability Analysis

This chapter deals with sustainability analysis of biorefinery systems in terms of environmental and socio-economic indicators. Life cycle analysis has methodological issues related to the functional unit (FU), allocation, land use and biogenic carbon neutrality of the reference system and of the biorefinery-based system. Socio-economic criteria and indicators used in sustainability frameworks assessment are presented and discussed. There is not one single methodology that can aptly cover the synergies of environmental, economic, social and governance issues required to assess the sustainable production and use of bioenergy systems. The perfect metric for environmental issues is not yet established and some researchers prefer to avoid high levels of uncertainty in life cycle assessment (LCA) methodology and adopt more physically quantifying methods like the annual basis carbon (ABC) method presented here. In addition to establishing the perfect metric, there are three types of uncertainty when building scenarios with biorefinery-based systems that must be regarded to have a more holistic point of view. This uncertainty is at the level of the concept, of the configuration and of the operation.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Imperial College London, Universidade de Sao Paulo
Authors: J. S. M. Silva, C. (Ekstern), Prunescu, R. M. (Intern), Gernaey, K. (Intern), Sin, G. (Intern), Diaz-Chavez, R. A. (Ekstern)
Bottom-Up Design of a Copper-Ruthenium Nanoparticulate Catalyst for Low-Temperature Ammonia Oxidation

A novel nanoparticulate catalyst of copper (Cu) and ruthenium (Ru) was designed for low-temperature ammonia oxidation at near-stoichiometric mixtures using a bottom-up approach. A synergistic effect of the two metals was found. An optimum CuRu catalyst presents a reaction rate threefold higher than that for Ru and forty-fold higher than that for Cu. X-ray absorption spectroscopy suggests that in the most active catalyst Cu forms one or two monolayer thick patches on Ru and the catalysts are less active once 3D Cu islands form. The good performance of the tuned Cu/Ru catalyst is attributed to changes in the electronic structure, and thus the altered adsorption properties of the surface Cu sites.
Brittle fracture of polymer transient networks

We study the fracture of reversible double transient networks, constituted of water suspensions of entangled surfactant wormlike micelles reversibly linked by various amounts of telechelic polymers. We provide a state diagram that delineates the regime of fracture without necking of the filament from the regime where no fracture or break-up has been observed. We show that filaments fracture when stretched at a rate larger than the inverse of the slowest relaxation time of the networks. We quantitatively demonstrate that dissipation processes are not relevant in our experimental conditions and that, depending on the density of nodes in the networks, fracture occurs in the linear viscoelastic regime or in a nonlinear regime. In addition, analysis of the crack opening profiles indicates deviations from a parabolic shape close to the crack tip for weakly connected networks. We demonstrate a direct correlation between the amplitude of the deviation from the parabolic shape and the amount of nonlinear viscoelasticity.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Universite de Montpellier, Laboratoire Charles Coulomb
Authors: Arora, S. (Ekstern), Shabbir, A. (Intern), Hassager, O. (Intern), Ligoure, C. (Ekstern), Ramos, L. (Ekstern)
Pages: 1267-1275
Brittle fracture of polymer transient networks

We study the fracture of reversible double transient networks, constituted of a water suspension of entangled surfactant wormlike micelles reversibly linked by various amounts of telechelic polymers. We provide a state diagram that delineates the regime of fracture without necking of the filament from the regime where no fracture or breakup has been observed. We show that filaments fracture when stretched at a rate larger than the inverse of the slowest relaxation time of the networks. We quantitatively demonstrate that dissipation processes are not relevant in our experimental conditions and that, depending on the density of nodes in the networks, fracture occurs in the linear elastic regime or in a nonlinear elastic regime. In addition, analysis of the crack opening profiles indicates deviations from a parabolic shape close to the crack tip for weakly connected networks. We demonstrate a direct relation between the amplitude of the deviation from the parabolic shape and the amount of non-linear elasticity.

Calculation of Multiphase Chemical Equilibrium by the Modified RAND Method

A robust and efficient algorithm for simultaneous chemical and phase equilibrium calculations is proposed. It combines two individual nonstoichiometric solving procedures: a nested-loop method with successive substitution for the first steps and final convergence with the second-order modified RAND method. The modified RAND extends the classical RAND method from single-phase chemical reaction equilibrium of ideal systems to multiphase chemical equilibrium of nonideal systems. All components in all phases are treated in the same manner and the system Gibbs energy can be used to monitor convergence. This is the first time that modified RAND was applied to multiphase chemical equilibrium systems. The combined algorithm was tested using nine examples covering vapor–liquid (VLE) and vapor–liquid–liquid equilibria (VLLE) of ideal and nonideal reaction systems. Successive substitution provided good initial estimates for the accelerated computation with modified RAND, to ultimately converge to the equilibrium solution without failure.
Calculation of simultaneous chemical and phase equilibrium by the method of Lagrange multipliers

The purpose of this work is to develop a general, reliable and efficient algorithm, which is able to deal with multiple reactions in multiphase systems. We selected the method of Lagrange multipliers to minimize the Gibbs energy of the system, under material balance constraints. Lagrange multipliers and phase amounts are the independent variables, whose initialization is performed by solving a subset of the working equations. This initialization is the unconstrained minimization of a convex function and it is bound to converge. The whole solution procedure employs a nested loop with Newton iteration in the inner loop and non-ideality updated in the outer loop, thus giving an overall linear convergence rate. Stability analysis is used to introduce additional phases sequentially so as to obtain the final multiphase solution. The procedure was successfully tested on vapor-liquid equilibrium (VLE) and vapor-liquid-liquid equilibrium (VLLE) of reaction systems.
Calibration of the comprehensive NDHA-\(\text{N}_2\text{O}\) dynamics model for nitrifier-enriched biomass using targeted respirometric assays

The NDHA model comprehensively describes nitrous oxide (N2O) producing pathways by both autotrophic ammonium oxidizing and heterotrophic bacteria. The model was calibrated via a set of targeted extant respirometric assays using enriched nitrifying biomass from a lab-scale reactor. Biomass response to ammonium, hydroxylamine, nitrite and N2O additions under aerobic and anaerobic conditions were tracked with continuous measurement of dissolved oxygen (DO) and N2O. The sequential addition of substrate pulses allowed the isolation of oxygen-consuming processes. The parameters to be estimated were determined by the information content of the datasets using identifiability analysis. Dynamic DO profiles were used to calibrate five parameters corresponding to endogenous, nitrite oxidation and ammonium oxidation processes. The subsequent N2O calibration was not significantly affected by the uncertainty propagated from the DO calibration because of the high accuracy of the estimates. Five parameters describing the individual contribution of three biological N2O pathways were estimated accurately (variance/mean < 10% for all estimated parameters). The NDHA model response was evaluated with statistical metrics (F-test, autocorrelation function). The 95% confidence intervals of DO and N2O predictions based on the uncertainty obtained during calibration are studied for the first time. The measured data fall within the 95% confidence interval of the predictions, indicating a good model description. Overall, accurate parameter estimation and identifiability analysis of ammonium removal significantly decreases the uncertainty propagated to N2O production, which is expected to benefit N2O model discrimination studies and reliable full scale applications.

General information
State: Published
Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Technical University of Denmark
Authors: Domingo-Felez, C. (Intern), Calderó-Pascual, M. (Ekstern), Sin, G. (Intern), Plósz, B. G. (Intern), Smets, B. F. (Intern)
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Camera Measurements in Cement Kilns – Impact of Alternative Fuels on Kiln Flames

Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Catalytic Science and Technology in Sustainable Energy II
This special issue of Catalysis Today results from four sessions, under the collective theme "Catalysis in Sustainable Energy", of the 2nd International Symposium on Catalytic Science and Technology in Sustainable Energy and Environment, held in Tianjin, China during October 12-14, 2016. This biennial symposium offers an international forum for discussing and sharing the cutting-edge researches and the most recent breakthroughs in energy and environmental technologies based on catalysis principles. Included in this special issue are 36 invited contributions, which is a noticeable expansion as compared with the 29 contributions published two years ago in the previous special issue of Catalysis Today under the same title "Catalytic Science and Technology in Sustainable Energy". We gratefully acknowledge all the authors and reviewers of the manuscripts and the editorial team of Elsevier, without whom the special issue would not have been possible. As the organizer of the EECAT 2016, Y Li expresses his special gratitude to the sponsors, especially Haldor Topsoe and Synfuels China, the participants and the co-organizers for their great contribution to the success of EECAT 2016.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Tianjin University, Zhejiang University, University of Twente, Aalto University
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.312 SNIP 1.363
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.316 SNIP 1.413 CiteScore 4
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.316 SNIP 1.474 CiteScore 3.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.307 SNIP 1.432 CiteScore 3.39
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.475 SNIP 1.437 CiteScore 3.38
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.479 SNIP 1.526 CiteScore 3.34
CFD Modeling of Flow and Ion Exchange Kinetics in a Rotating Bed Reactor System

A rotating bed reactor (RBR) has been modeled using computational fluid dynamics (CFD). The flow pattern in the RBR was investigated and the flow through the porous material in it was quantified. A simplified geometry representing the more complex RBR geometry was introduced and the simplified model was able to reproduce the main characteristics of the flow. Alternating reactor shapes were investigated, and it was concluded that the use of baffles has a very large impact on the flows through the porous material. The simulations suggested, therefore, that even faster reaction rates could be achieved by making the baffles deeper. Two-phase simulations were performed, which managed to reproduce the deflection of the gas–liquid interface in an unbaffled system. A chemical reaction was implemented in the model, describing the ion-exchange phenomena in the porous material using four different Sherwood number correlations. The simulations were overall in good agreement with experimental data.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark, SpinChem AB
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Pages: 3853–3865
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.342 SNIP 1.398
CFD simulations on marine burner flames
The marine industry is changing with new demands concerning high energy efficiency, fuel flexibility and lower emissions of NOX and SOX. A collaboration between the company Alfa Laval and Technical University of Denmark has been established to support the development of the next generation of marine burners. The resulting auxiliary boilers shall be compact and able to operate with different fuel types, while reducing NOX emissions.

The specific boiler object of this study uses a swirl stabilized liquid fuel burner, with a pressure swirl spill-return atomizer (Fig.1). The combustion chamber is enclosed in a water jacket used for water heating and evaporation, and a convective heat exchanger at the furnace outlet super-heats the steam.

The purpose of the present study is to gather detailed knowledge about the influence of fuel spray conditions on marine utility boiler flames. The main goal of work presented in this paper was to obtain a spray description to setup a particle injection region in the CFD simulations of the boiler.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST)
Authors: Cafaggi, G. (Intern), Jensen, P. A. (Intern), Glarborg, P. (Intern), Clausen, S. (Intern), Dam-Johansen, K. (Intern)
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Changes imposed by pyrolysis, thermal gasification and incineration on composition and phosphorus fertilizer quality of municipal sewage sludge
Fertilizer quality of ash and char from incineration, gasification and pyrolysis of a single municipal sewage sludge sample were investigated by comparing composition and phosphorus (P) plant availability. A process for post oxidation of gasification ash and pyrolysis char was developed and the oxidized materials were investigated as well. Sequential extraction with full elemental balances of the extracted pools as well as scanning electron microscopy with energy dispersive X-ray spectroscopy were used to investigate the mechanisms driving the observed differences in composition and P plant availability in a short-term soil incubation study. The compositional changes related mainly to differences in the proximate composition as well as to the release of especially nitrogen, sulfur, cadmium and to some extent, phosphorus (P). The cadmium load per unit of P was reduced with 75–85% in gasification processes and 10–15% in pyrolysis whereas no reduction was observed in incineration processes. The influence on other heavy metals was less pronounced. The plant availability of P in the substrates varied from almost zero to almost 100% of the plant availability of P in the untreated sludge. Post-oxidized slow pyrolysis char was found to be the substrate with the highest P fertilizer value while ash from commercial fluid bed sludge incineration had the lowest P fertilizer quality. The high P fertilizer value in the best substrate is suggested to be a function of several different mechanisms including structural surface changes and improvements in the association of P to especially magnesium, calcium and aluminum.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Copenhagen
Authors: Thomsen, T. P. (Intern), Sárossy, Z. (Intern), Ahrenfeldt, J. (Intern), Henriksen, U. B. (Intern), Jappe Frandsen, F. (Intern), Müller-Stöver, D. S. (Ekstern)
Pages: 308-318
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Chapter 3 – VPPD-Lab: The Chemical Product Simulator

Computer-aided methods and tools for current and future product-process design and development need to manage problems requiring efficient handling of models, data, and knowledge from different sources and at different times and size scales. In this chapter, a systematic model-based framework for computer-aided chemical product design and evaluation, implemented in the software called VPPD-Lab, is presented. In the same way a typical process simulator works, the VPPD-Lab allows users to: (1) analyze chemical-based products by performing virtual experiments (product property and...
performance calculations), (2) predict the properties of products, and (3) create new product property and product performance models when needed. However, unlike process simulators, VPPD-Lab can also be used directly for (1) design of chemicals based products using design templates for various types of products, such as single molecule products, formulations, blends, emulsions, and devices; and (2) to create new product design templates when the needed template for a desired product is not available. VPPD-Lab employs a suite of algorithms (such as database search, molecular and mixture blend design) and toolboxes (such as property calculations and property model consistency tests) for specific product property prediction, design, and/or analysis tasks. The application of VPPD-Lab is highlighted through case studies involving solvent mixture stability check, lubricant blend design, jet fuel blend design, and insect repellent lotion design. Through these case studies, the use of design templates, associated workflows (methods), data flows (software integration), and solution strategies (database and tools) are highlighted.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, Hong Kong University of Science and Technology
Authors: Kalakul, S. (Intern), Cignitti, S. (Intern), Zhang, L. (Ekstern), Gani, R. (Intern)
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Chapter 6 – Computer-Aided Molecular Design and Property Prediction
Today’s society needs many chemical-based products for its survival, nutrition, health, transportation, agriculture, and the functioning of processes. Chemical-based products have to be designed/developed in order to meet these needs, while at the same time, they must be innovative and sustainable to meet the global challenges of resources, competition, and demand. Design/development of these products mostly follows experiment-based trial and error approaches. With the availability of reliable property prediction models, however, computer-aided techniques have become popular, at least for the initial stages of the design/development process. Therefore, computer-aided molecular design and property prediction techniques are two topics that play important roles in chemical product design, analysis, and application. In this chapter, an overview of the concepts, methods, and tools related to these two topics are given. In addition, a generic computer-aided framework for the design of molecules, mixtures, and blends is presented. The application of the framework is highlighted for molecular products through two case studies involving the design of refrigerants and surfactants.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, Technical University of Denmark
Authors: Gani, R. (Intern), Zhang, L. (Ekstern), Kalakul, S. (Intern), Cignitti, S. (Intern)
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ISBN (Print): 978-0-444-63683-6
Characterisation of Authentic Lignin Biorefinery Samples by Fourier Transform Infrared Spectroscopy and Determination of the Chemical Formula for Lignin

Efficient methods for lignin characterisation are increasingly important as the field of lignin valorisation is growing with the increasing use of lignocellulosic feedstocks, such as wheat straw and corn stover, in biorefineries. In this study, we characterised a set of authentic lignin biorefinery samples in situ with no prior purification and minimal sample preparation. Lignin chemical formulas and lignin Fourier transform infrared (FTIR) spectra were extracted from mixed spectra by filtering out signals from residual carbohydrates and minerals. From estimations of C, H and O and adjustment for cellulose and hemicelluloses contents, the average chemical formula of lignin was found to be C9H10.2O3.4 with slight variations depending on the biomass feedstock and processing conditions (between C9H9.5O2.8 and C9H11.1O3.6). Extracted FTIR lignin spectra showed many of the same characteristic peaks as organosolv and kraft lignin used as benchmark samples. Some variations in the lignin spectra of biorefinery lignin residue samples were found depending on biomass feedstock (wheat straw, corn stover or poplar) and on pretreatment severity, especially in the absorbance of bands at 1267 and 1032 cm\(^{-1}\) relative to the strong band at \(\sim 1120\) cm\(^{-1}\). The suggested method of FTIR spectral analysis with adjustment for cellulose and hemicellulose is proposed to provide a fast and efficient way of analysing lignin in genuine lignin samples resulting from biorefineries.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DONG Energy A/S, Technical University of Denmark
Authors: Le, D. M. (Intern), Damgaard Nielsen, A. (Ekstern), Sørensen, H. (Ekstern), Meyer, A. S. (Intern)
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Scopus rating (2016): CiteScore 2.64 SJR 0.943 SNIP 0.932
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.317 SNIP 1.285 CiteScore 3.35
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.453 SNIP 1.344 CiteScore 3.64
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.162 SNIP 1.384 CiteScore 3.66
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 1.362 SNIP 1.645 CiteScore 4.23
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 1 SNIP 1.435 CiteScore 3.16
A sialidase (EC 3.2.1.18; GH 33) from non-pathogenic Trypanosoma rangeli has been engineered with the aim of improving its transsialylation activity. Recently, two engineered variants containing 15 and 16 amino acid substitutions, respectively, were found to exhibit significantly improved transsialylation activity: both had a 14 times higher ratio between transsialylation and hydrolysis products compared to the first reported mutant TrSA5mut. In the current work, these two variants, Tr15 and Tr16, were characterized in terms of pH optimum, thermal stability, effect of acceptor-to-donor ratio, and acceptor specificity for transsialylation using casein glycomacropeptide (CGMP) as sialyl donor and lactose or other human milk oligosaccharide core structures as acceptors. Both sialidase variants exhibited pH optima around pH 4.8.

Thermal stability of each enzyme was comparable to that of previously developed T. rangeli sialidase variants and higher than that of the native transsialidase from T. cruzi (TcTS). As for other engineered T. rangeli sialidase variants and TcTS, the acceptor specificity was broad: lactose, galactooligosaccharides (GOS), xylooligosaccharides (XOS), and human milk oligosaccharide structures lacto-N-tetraose (LNT), lacto-N-fucopentaose (LNFP V), and lacto-N-neofucopentaose V (LNnFP V) were all sialylated by Tr15 and Tr16. An increase in acceptor-to-donor ratio from 2 to 10 had a positive effect on transsialylation. Both enzymes showed high preference for formation α(2,3)-linkages at the non-reducing end of lactose in the transsialylation. Tr15 was the most efficient enzyme in terms of transsialylation reaction rates and yield of 3'-sialyllactose. Finally, Tr15 was immobilized covalently on glyoxyl-functionalized silica, leading to a 1.5-fold increase in biocatalytic productivity (mg 3'-sialyllactose per mg enzyme) compared to free enzyme after 6 cycles of reuse. The use of glyoxyl-functionalized silica proved to be markedly better for immobilization than silica functionalized with (3-aminopropyl)triethoxysilane (APTES) and glutaraldehyde, which resulted in a biocatalytic productivity which was less than half of that obtained with free enzyme.
Characterization of a continuous agitated cell reactor for oxygen dependent biocatalysis

Biocatalytic oxidation reactions employing molecular oxygen as the electron acceptor are difficult to conduct in a continuous flow reactor because of the requirement for high oxygen transfer rates. In this paper, the oxidation of glucose to glucono-1,5-lactone by glucose oxidase was used as a model reaction to study a novel continuous agitated cell reactor (ACR). The ACR consists of ten cells interconnected by small channels. An agitator is placed in each cell, which mixes the content of the cell when the reactor body is shaken by lateral movement. Based on tracer experiments, a hydrodynamic model for the ACR was developed. The model consisted of ten tanks-in-series with back-mixing occurring within and between each cell. The back-mixing was a necessary addition to the model in order to explain the observed phenomenon that the ACR behaved as two continuous stirred tank reactors (CSTRs) at low flow rates, while it at high flow rates behaved as the expected ten CSTRs in series. The performance of the ACR was evaluated by comparing the steady state conversion at varying residence times with the conversion observed in a stirred batch reactor of comparable size. It was found that the ACR could more than double the overall reaction rate, which was solely due to an increased oxygen transfer rate in the ACR caused by the intense mixing as a result of the spring agitators. The volumetric oxygen transfer coefficient, kL a, was estimated to be 344 h⁻¹ in the 100mL ACR, opposed to only 104 h⁻¹ in a batch reactor of comparable working volume. Interestingly, the large deviation from plug flow behavior seen in the tracer experiments was found to have little influence on the conversion in the ACR, since both a plug flow reactor (PFR) model and the backflow cell model described the data sufficiently well. Biotechnol. Bioeng. 2017;9999: 1-9. © 2017 Wiley Periodicals, Inc.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, AM Technology
Authors: Pedersen, A. T. (Intern), Teresa de Melo Machado Simoes Carvalho, A. (Intern), Sutherland, E. (Ekstern), Rehn, G. (Intern), Ashe, R. (Ekstern), Woodley, J. (Intern)
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Scopus rating (2016): CiteScore 4.14 SJR 1.411 SNIP 1.163
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.589 SNIP 1.401 CiteScore 4.16
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.621 SNIP 1.425 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.639 SNIP 1.366 CiteScore 4.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.668 SNIP 1.483 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
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Characterization of alginates from Ghanaian brown seaweeds: Sargassum spp. and Padina spp

Alginates of four locally harvested Ghanaian brown seaweeds from the Sargassum and Padina genus were assessed for their rheological and chemical characteristics. The seaweeds contained 16–30% by weight of alginate assessed as the sum of d-mannuronic acid (M) and l-guluronic acid (G). In comparison, alginate samples from Laminaria digitata and Macrocystis pyrifera, used commercially for alginate extraction, contained 29% and 27% by weight of the two constituent uronic acids (M + G), respectively. Alginate extraction yields of the Ghanaian seaweeds ranged from 17 to 23% by weight of dry material; the corresponding yields from L. digitata and M. pyrifera were 26–29% by weight; these yields were equivalent to ~49–99% of the theoretical yields, but the purity of the extracted alginates varied, and were lowest for the Ghanaian seaweed alginates. 1H NMR analysis of the uronic acid block-structure in the alginates gave M/G ratios of 0.47 and 0.70 for the alginates extracted from Sargassum natans and Sargassum vulgare, while alginates from Padina gymnospora and Padina antillarum had M/G ratios of 1.75 and 1.85, respectively. The alginates from the two Ghanaian Sargassum spp. had high contents of dimeric and trimeric homoguluronate elements: $F_{GG}$ and $F_{GGG}$ values were 0.61 and 0.58 for S. natans and 0.49 and 0.44 for S. vulgare. The alginates from the two Padina spp. had gel strengths estimated as G’ surpassing those from the commercial alginates with G’ values after 4 h of rheological oscillation of 340 Pa (P. gymnospora) and 376 Pa (P. antillarum), whereas the gelling properties of the Sargassum spp. alginates were poor. The degree of polymerization of the acid tolerant alginate backbone fragments, but not M/G ratio or homoguluronate dimer and trimer element contents, appeared to correlate to the alginate gel strength. The study shows that notably Ghanaian Padina spp. hold alginate having desirable properties for high gel-strength applications.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, National Food Institute, Research Group for Nano-Bio Science
Authors: Rhein-Knudsen, N. (Intern), Ale, M. T. (Intern), Ajalloueian, F. (Intern), Meyer, A. S. (Intern)
Pages: 236-244
Characterization of two novel bacterial type A exo-chitobiose hydrolases having C-terminal 5/12-type carbohydrate-binding modules

Type A chitinases (EC 3.2.1.14), GH family 18, attack chitin (\((1 \rightarrow 4)\)-2-acetamido-2-deoxy-\(\beta\)-D-glucan) and chito-oligosaccharides from the reducing end to catalyze release of chitobiose (N,N'-diacetylchitobiose) via hydrolytic cleavage of N-acetyl-\(\beta\)-D-glucosaminide (1 \(\rightarrow\) 4)-\(\beta\)-linkages and are thus "exo-chitobiose hydrolases." In this study, the chitinase type A from Serratia marcescens (SmaChiA) was used as a template for identifying two novel exo-chitobiose hydrolase type A enzymes, FbalChi18A and MvarChi18A, originating from the marine organisms Ferrimonas balearica and Microbulbifer variabilis, respectively. Both FbalChi18A and MvarChi18A were recombinantly expressed in Escherichia coli and were confirmed to exert exo-chitobiose hydrolase activity on chito-oligosaccharides, but differed in temperature and pH activity response profiles. Amino acid sequence comparison of the catalytic \(\beta/\alpha\) barrel domain of each of the new enzymes showed individual differences, but ~69% identity of each to that of SmaChiA and highly conserved active site residues. Superposition of a model substrate on 3D structural models of the catalytic domain of the enzymes corroborated exo-chitobiose hydrolase type A activity for FbalChi18A and MvarChi18A, i.e., substrate attack from the reducing end. A main feature of both of the new enzymes was the presence of C-terminal 5/12 type carbohydrate-binding modules (SmaChiA has no C-terminal carbohydrate binding module). These new enzymes may be useful tools for utilization of chitin as an N-acetylglucosamine donor substrate via chitobiose.

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
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Scopus rating (2016): CiteScore 3.57 SJR 1.177 SNIP 1.173
Web of Science (2016): Indexed yes
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.327 SNIP 1.458 CiteScore 3.71
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.533 SNIP 1.432 CiteScore 4.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.507 SNIP 1.286 CiteScore 4
ISI indexed (2012): ISI indexed yes
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Scopus rating (2011): SJR 1.437 SNIP 1.232 CiteScore 3.72
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Chemically extracted nanocellulose from sisal fibres by a simple and industrially relevant process

A novel type of acetylated cellulose nanofibre (CNF) was extracted successfully from sisal fibres using chemical methods. Initially, a strong alkali treatment was used to swell the fibres, followed by a bleaching step to remove the residual lignin and finally an acetylation step to reduce the impact of the intermolecular hydrogen bonds in the nanocellulose. The result of this sequence of up-scalable chemical treatments was a pulp consisting mainly of micro-sized fibres, which allowed simpler handling through filtration and purification steps and permitted the isolation of an intermediate product with a high solids content. An aqueous dispersion of CNF could be obtained directly from this intermediate pulp by simple magnetic stirring. As a proof of concept, the dispersion was used directly for preparing a highly translucent CNF film, illustrating that there are no large aggregates in the prepared CNF dispersion. Finally, CNF films with alkali extracts were also prepared, resulting in flatter films with an increased mass yield and improved mechanical strength.

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Organisations: The Danish Polymer Centre, Department of Mechanical Engineering, Manufacturing Engineering, Department of Chemical and Biochemical Engineering, University of British Columbia, Grenoble-INP Pagora
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Clean Cook Stove Technology for Artisanal Palm Oil Clarification and Biochar Production in Ghana

The method of heat provision for artisanal palm oil production in Ghana is riddled with inefficient systems which create unfavourable working conditions (use of spent tyres, smoke filled work tents etc.) for the women who engage in this process. This creates health hazards for the women and sometimes the children they carry along to work. This study, therefore, sought to produce a cook stove that provides a healthy work environment, is efficient, easy to use, and affordable for medium-scale clarification of palm oil. Further it should have a sustainable source of fuel (biomass from
processing the palm fruits) and simultaneously produce heat and biochar. The adopted design procedure was iterative and eight preliminary tests were conducted; each an improvement of the previous stove tested. The best stove configuration was adopted for the design calculations and the final stove fabricated and tested. The fabricated stove consisted mainly of a cut out barrel, a chimney and a grate. The stove was insulated to improve its thermal efficiency. Water boiling tests and controlled cooking tests protocols were adopted for the evaluation of the stove. The thermal efficiency of the stove was calculated to be $33 \pm 7\%$ thus representing a 400% increase in efficiency as compared with the local replica stove. The cook stove was able to process approximately 103 litres of press liquor into 35 litres of palm oil within 55 minutes for one cycle of clarification. The quantity of fuel mix used was 9.5 kg with a biochar yield of 5%. A maximum CO emission of 5 ppm was measured. The study showed that the palm oil clarification process with the designed cook stove provided a smokeless work environment, heat and biochar.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Kwame Nkrumah University of Science and Technology, University of Ghana, Aarhus University
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Cook stove, Biomass, CO emission, Palm fruit fibre, Palm kernel shell, Bio char
Publication: Research › Paper – Annual report year: 2018

**Closing the Loop for Packaging: Finding a Framework to Operationalize Circular Economy Strategies**

This paper examines some of the most common frameworks available to companies in implementing circular economy strategies, i.e. the Cradle-to-Cradle design protocol, the Material Circularity Indicator and the Life Cycle Sustainability Assessment framework intended as a combination of Life Cycle Assessment, Environmental Life Cycle Costing and Social Life Cycle Assessment. We focus on the packaging sector and use the case of closed-loop aluminium can supply to illustrate the benefits and limitations of combining some of these frameworks. Our recommendation is to use the Life Cycle Sustainability Assessment framework to evaluate circularity strategies, since it is the most comprehensive and still operational framework and best at preventing burden shifting between stakeholders in the value chain.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Niero, M. (Intern), Hauschild, M. Z. (Intern)
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Control and Systems Engineering, Industrial and Manufacturing Engineering, aluminium, circularity, cradle to cradle, environmental Life Cycle Costing, Life Cycle Assessment, Life Cycle Sustainability Assessment, life cycle thinking, material circularity indicator, Social LCA, Aluminum, Network function virtualization, Sustainable development, Cradle to cradles, Environmental life cycle, Life Cycle Assessment (LCA), Life cycle sustainability assessments, Life cycle thinking, Life cycle
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CO2 Capture with Liquid-Liquid Phase Change Solvents: A Thermodynamic Study

Extended UNIQUAC thermodynamic framework was implemented in this work to model the aqueous blend of N, N-Diethylethanolamine (DEEA) and N-Methyl-1,3-diaminopropane (MAPA) for CO2 capture. The model parameters were estimated first for the two ternary systems, H2O-DEEA-CO2 and H2O-MAPA-CO2, followed by the quaternary H2O-DEEAMAPA-CO2 system which gives liquid-liquid phase split when reacted with carbon dioxide. A total of 94 model parameters and 6 thermodynamic properties were fitted to approximately 1500 equilibrium and thermal experimental data consisting of pureamine vapor pressure (Pvap), vapor-liquid equilibrium (VLE), solid-liquid equilibrium (SLE), liquid-liquid equilibrium (LLE), excess enthalpy (HEx), and heat of absorption (ΔHabs) of CO2 in aqueous amine solutions. The model developed in this work can accurately represent the equilibrium and thermal data for the studied systems with a single unique set of parameters.
Comparison of GERG-2008 and simpler EoS models in calculation of phase equilibrium and physical properties of natural
gas related systems

Accurate description of thermodynamic properties of natural gas systems is of great significance in the oil and gas
industry. For this application, non-cubic equations of state (EoSs) are advantageous due to their better density and
compressibility description. Among the non-cubic models, GERG-2008 is a new wide-range EoS for natural gases and
other mixtures of 21 natural gas components. It is considered as a standard reference equation suitable for natural gas
applications where highly accurate thermodynamic properties are required. Soave’s modification of Benedict-Webb-Rubin
(Soave-BWR) EoS is another model that despite its empirical nature, provides accurate density description even around
the critical point. It is much simpler than GERG-2008 and easier to handle and generalize to reservoir oil fluids. This study
presents a comprehensive comparison between GERG-2008 and other cubic (SRK and PR) and noncubic EoSs (Soave-
BWR and PC-SAFT) with a focus on Soave-BWR in description of pure components density and compressibility in a wide
temperature and pressure range, calculation of binary Vapor-Liquid-Equilibria (VLE) and density, prediction of
multicomponent phase envelopes and gas compressibility factor. In addition, the performance of GERG-2008 is compared
with that of cubic and non-cubic models in calculation of thermal properties such as heat capacity and Joule-Thomson
coefficient for pure components and multicomponent mixtures over a wide pressure and temperature range. The results
are compared with available experimental data in the literature and special emphasis has been given to the reverse Joule-
Thomson effects at high pressure high temperature (HPHT) conditions. © 2016 Elsevier B.V. All rights reserved.

General information
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Organisations: Department of Chemistry, Center for Energy Resources Engineering, Department of Chemical and
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Authors: Varzandeh, F. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
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Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Comparison of phosphorus recovery from incineration and gasification sewage sludge ash

Incineration of sewage sludge is a common practice in many western countries. Gasification is an attractive option because of its high energy efficiency and flexibility in the usage of the produced gas. However, they both unavoidably produce sewage sludge ash (SSA), a material which is rich in phosphorus (P), but that it is commonly landfilled or used in construction materials. With current uncertainty in phosphate rock (PR) supply, P recovery from SSA has become interesting. In the present work, ashes from incineration and gasification of the same sewage sludge were compared in terms of P extractability using electrodialytic (ED) methods. The results show that comparable recovery rates of P were achieved with a single ED step for incineration SSA and a sequential combination of two ED steps for gasification SSA, which was due to a higher influence of Fe and/or Al in P solubility for the latter. A product with lower level of metallic impurities and comparable to wet process phosphoric acid (WPA) was eventually obtained from gasification SSA. Thus, gasification becomes an interesting alternative to incineration also in terms of P separation.

General information
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Organisations: Department of Civil Engineering, ARTEK, Section for Arctic Engineering and Sustainable Solutions, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Roskilde University
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.394 SNIP 0.621
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.466 SNIP 0.599 CiteScore 1.19
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.587 SNIP 0.685 CiteScore 1.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.568 SNIP 0.7 CiteScore 1.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.601 SNIP 0.669 CiteScore 1.13
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.591 SNIP 0.626 CiteScore 1.25
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.522 SNIP 0.602
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.589 SNIP 0.686
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.579 SNIP 0.697
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.749 SNIP 0.781
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.693 SNIP 0.796
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.763 SNIP 0.85
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.877 SNIP 0.904
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.882 SNIP 0.902
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.903 SNIP 0.888
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.759 SNIP 0.967
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.76 SNIP 0.885
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.889 SNIP 0.936
Original language: English
Electrodialysis, Heavy metals, Incineration, Low-temperature gasification, Phosphorus, Sewage sludge ash
Comparison of the Kinetic Promoters Piperazine and Carbonic Anhydrase for CO₂ Absorption

Kinetic promoter that enhance the reaction kinetics with CO₂ are enabling the use of the low heat of reaction of slow absorbing solvents like MDEA. Mass transfer experiments with 30 wt% MDEA promoted by either by 1.7 and 8.5g/L enzyme carbonic anhydrase (CA) or 5 wt% piperazine (PZ) where conducted in a wetted wall column apparatus at 298, 313K and 328 for different solvent loadings. The mass transfer of PZ promoted solvents was strongly influenced by the solvent loading as it was steeply decreasing for all temperatures; the temperature was also influencing the mass transfer, but the extent was dependent on the solvent loading. CA promoted solvent mass transfer characteristics showed less dependency on the solvent loading and temperature. Lower enzyme concentrations were found to be much slower than MDEA/PZ solvents, whereas high enzyme concentrations might be as efficient in capturing CO₂ as a 30 wt% MDEA/5 wt% PZ mixture in terms of overall mass transfer, considering change of mass transfer due to solvent loading over the height of a column.

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
Authors: Gladis, A. (Intern), Gundersen, M. T. (Intern), Thomsen, K. (Intern), Fosbøl, P. L. (Intern), Woodley, J. M. (Intern), von Solms, N. (Intern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.365 SNIP 0.561 CiteScore 0.92
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.433 SNIP 0.81 CiteScore 1.09
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.425 SNIP 0.785 CiteScore 1.02
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.433 SNIP 0.957
Web of Science (2009): Indexed yes
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Piperazine, MDEA, Carbonic anhydrase, Wetted wall column
Electronic versions:
Comparison_of_the_kinetic_promoters.pdf
Comparison of traditional field retting and Phlebia radiata Cel 26 retting of hemp fibres for fibre-reinforced composites

Classical field retting and controlled fungal retting of hemp using Phlebia radiata Cel 26 (a mutant with low cellulose degrading ability) were compared with pure pectinase treatment with regard to mechanical properties of the produced fibre/epoxy composites. For field retting a classification of the microbial evolution (by gene sequencing) and enzyme profiles were conducted. By phylogenetic frequency mapping, different types of fungi, many belonging to the Ascomycota phylum were found on the fibres during the first 2 weeks of field retting, and thereafter, different types of bacteria, notably Proteobacteria, also proliferated on the field retted fibres. Extracts from field retted fibres exhibited high glucanase activities, while extracts from P. radiata Cel 26 retted fibres showed high polygalacturonase and laccase activities. As a result, fungal retting gave a significantly higher glucan content in the fibres than field retting (77 vs. 67%) and caused a higher removal of pectin as indicated by lower galacturonan content of fibres (1.6%) after fibres were retted for 20 days with P. radiata Cel 26 compared to a galacturonan content of 3.6% for field retted fibres. Effective fibre stiffness increased slightly after retting with P. radiata Cel 26 from 65 to 67 GPa, while it decreased after field retting to 52 GPa. Effective fibre strength could not be determined similarly due to variations in fibre fracture strain and fibre-matrix adhesion. A maximum composite strength with 50 vol% fibres of 307 MPa was obtained using P. radiata Cel 26 compared to 248 MPa with field retting.

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Scopus rating (2016): CiteScore 2.15 SJR 0.65 SNIP 0.799
Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 1
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.589 SNIP 0.924 CiteScore 1.19
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.38 SNIP 0.953 CiteScore 1.06
ISI indexed (2012): ISI indexed no
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Original language: English
Hemp fibre, Field retting, Phlebia radiata Cel 26, Microbial community, Enzyme profiling, Composite strength
Electronic versions:
art_3A10.1186_2Fs13568_017_0355_8.pdf
DOIs:
10.1186/s13568-017-0355-8
Complementary Methods for the Characterization of Corrosion Products on a Plant-Exposed Superheater Tube

In this work, complex corrosion products on a superheater tube exposed to biomass firing were characterized by the complementary use of energy-dispersive synchrotron diffraction, electron microscopy, and energy-dispersive X-ray spectroscopy. Non-destructive synchrotron diffraction in transmission geometry measuring with a small gauge volume from the sample surface through the corrosion product allowed depth-resolved phase identification and revealed the presence of (Fe,Cr)₂O₃ and FeCr₂O₄. This was supplemented by microstructural and elemental analysis correlating the additional presence of a Ni-rich austenite phase to selective removal of Fe and Cr from the alloy, via a KCl-induced corrosion mechanism. Compositional variations were related to diffraction results and revealed a qualitative influence of the spinel cation concentration on the observed diffraction lines.

Complete mitochondrial genome of the Oriental Hornet, Vespa orientalis F. (Hymenoptera: Vespidae)

The Oriental Hornet (Vespa orientalis) is a social insect belonging to the Vespialde family (Wasps, Hornets, Yellowjackets), genus Vespa (true Hornets). The oriental hornet is a scavenger and an agricultural pest, especially to bee farmers, but is also recently described as a harvester of solar energy. Here, we report the mitochondrial genome sequence of the Oriental Hornet, Vespa orientalis F., which may play a vital role in understanding this wasp biology, light trapping and generation of electricity. The mitochondrial genome of this hornet is 16,099 bp in length, containing 13 protein-coding genes, 21 transfer RNA genes, and 2 ribosomal RNA genes. The overall base composition of the heavy-strand is 40.3% A, 5.9% C, 13.2% G, and 40.6% T, the percentages of A and T being higher than that of G and C. The mitochondrial genome of the Oriental Hornet, Vespa orientalis F., represents the first mitogenome of a solar energy harvesting insect.
Compositional variations of brown seaweeds Laminaria digitata and Saccharina latissima in Danish waters

Around Denmark, Laminaria digitata and Saccharina latissima are particularly common macroalgae species and are considered as prospective candidates for biorefineries. In this study, the carbohydrate composition and protein levels of L. digitata and S. latissima from three different sites in Denmark were compared for 1 year, and compositional variations of wild L. digitata harvested in August from the North Sea was monitored for 3 years. Glucan levels of L. digitata were consistently higher than those of S. latissima irrespective of harvest site and time of the year. Glucan levels in wild L. digitata from Kattegat peaked in October with 37.0% by dry weight compared to 22.6% by dry weight in wild S. latissima (Kattegat) and were accompanied by lower ash contents (18.5% w/w in L. digitata versus 26.5% w/w in S. latissima). Alginate contents were almost constant throughout the year, but mannuronic/glucuronic acid ratios differed between species and location from 1.33 to 3.64. Wild L. digitata harvested from the North Sea in August contained >50% glucans by weight and had low ash contents for three consecutive years (2012-2014). Compositional variation of the seaweeds was mainly related to season but also varied with species, location, and within populations. Among environmental variables (temperature, salinity, phosphate, nitrate, ammonia), only temperature was found to correlate with the chemical composition of the seaweeds. Amino acid profiles were dominated by glutamic acid, aspartic acid, and alanine and varied with season, especially for L. digitata from the North Sea, and location. Total nitrogen contents fluctuated more between samples than the actual protein contents; hence, application of a common N-to-protein factor cannot be recommended.
Computational chemical product design problems under property uncertainties

Three different strategies of how to combine computational chemical product design with Monte Carlo based methods for uncertainty analysis of chemical properties are outlined. One method consists of a computer-aided molecular design (CAMD) solution and a post-processing property uncertainty propagation through the considered process. It is demonstrated for an industrial case study on identification of a suitable working fluid in a thermodynamic cycle for waste heat recovery. The results show that including property uncertainties gives an additional criterion for the fluid ranking in working fluid design. While the higher end of the uncertainty range of the process model output is similar for the best performing fluids, the lower end of the uncertainty range differs largely.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Frutiger, J. (Intern), Cignitti, S. (Intern), Abildskov, J. (Ekstern), Woodley, J. (Intern), Sin, G. (Intern)
Computational Fluid Dynamics - en genvej til procesindsigt
I artiklen gives der tre konkrete eksempler på, hvordan CFD kan bruges til at opnå procesindsigt på nuværende anlæg og på processer i udviklingsfasen.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Novozymes A/S
Authors: Bach, C. (Intern), Spann, R. (Intern), Larsson, H. K. (Intern), Pereira Rosinha Grundtvig, I. (Intern), Albæk, M. O. (Ekstern), Gernaey, K. V. (Intern), Krühne, U. (Intern)
Pages: 14-17
Publication date: 2017
Main Research Area: Technical/natural sciences

Computer Aided Synthesis of Innovative Processes: Renewable Adipic Acid Production
A promising biotechnological route for the production of adipic acid from renewables has been evaluated, applying a systematic methodology for process network synthesis and optimization. The method allows organizing in a structured database the available knowledge from different sources (preliminary scientific studies, techno-economic process specifications), generating a network of process alternatives and solving it as a MILP. The best processing route provides also an estimate of the production cost of bio-adipic acid at the current state of the art, assessing the sensitivity of the results to the change of the production scenarios (e.g. improvement of bacterial productivity). Thus, this method can support R&D strategy definition, targeting the research efforts on precise short-term objectives, set by the full-scale process feasibility.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre, Technical University of Denmark, Politecnico di Milano
Considerations for implementation of novel enzyme-based processes

Biocatalysis is the use of enzymes to catalyze chemical reactions. It is an established synthesis route in chemical synthesis, alongside conventional chemistry. Biocatalysis is often applied due to excellent regio and stereoselectivity, in addition to its environmentally benign properties. This thesis aims at increasing the potential use of industrial biocatalysis, both in terms of broadening its current use and expanding it to new applications. This academic study is carried out through two case studies. These two case studies were chosen because they represent each end of the spectra of biocatalytic applications. The first case study is expanding the use of an established biocatalyst. The second case study investigates the potential of a novel biocatalyst. In addition, the two case studies have very different implementation challenges, impeding current use. Therefore, arguably, the lessons learned from these two case studies justify general conclusions for biocatalysis, irrespective of their application. The work in this thesis therefore contributes, not only to industrial biocatalysis in these two areas, but also increases the understanding of biocatalysis as a whole.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium, CERE – Center for Energy Resources Engineering
Authors: Deslauriers, M. G. (Intern), Woodley, J. (Intern), von Solms, N. (Intern)
Number of pages: 203
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Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: 711866_DTU_PhD_Maria_Gundersen_Deslauriers_enkeltsider_til_orbit.pdf

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Projects:

Source: PublicationPreSubmission
Source-ID: 140201225
Publication: Research › Ph.D. thesis – Annual report year: 2017

Constant interchain pressure effect in extensional flows of oligomer diluted polystyrene and poly(methyl methacrylate) melts

The constant ‘interchain pressure’ idea has been addressed, to evaluate if it is an adequate quantitative assumption to describe the fluid mechanics of oligomer diluted entangled NMMD polymer systems. The molecular stress function constitutive framework has been used with the constant interchain pressure assumption. Furthermore, the maximal extensibility based on the number of Kuhn steps in an entanglement has been used based on the relative Padé inverse Langevin function. The model predictions agree with the extensional measurements on all previously published poly(methyl methacrylate)s and almost all published oligomer diluted NMMD polystyrenes. The only deviation is on the
most diluted and largest molecular weight case of an 18% 1880 kg/mol polystyrene in oligomer diluent. In this case, the maximal extensibility is not needed.
Continuous fermentation and kinetic experiments for the conversion of crude glycerol derived from second-generation biodiesel into 1,3 propanediol and butyric acid

This study investigated the performance of different mixed microbial cultures (MMC) able to ferment crude glycerol generated from animal fat-based biodiesel to produce 1,3 propanediol (1,3 PDO) and butyric acid, under non-sterile conditions. Eight different continuous flow stirred-tank reactors (CSTR) were set up with different inoculum types and growth media. The distribution of metabolic products under variable operating conditions was determined. All MMC were characterized from a kinetic point of view and overall stoichiometric reactions were constructed. Changes in the microbial communities were monitored by means of Next Generation Sequencing (NGS). Maximum substrate degradation rate reached approximately 110 g/L/d of glycerol (with a productivity of 38 g/L/d and 11 g/L/d for 1,3 PDO and butyric acid, respectively), obtained with an hydraulic retention time of 12 h and 60 g/L feed. The maximum feed concentration reached almost 90 g/L, leading though to an incomplete substrate degradation.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, PILOT PLANT, SINTEF, Technical University of Denmark
Authors: Varrone, C. (Intern), Floriotis, G. (Ekstern), Heggeset, T. M. B. (Ekstern), Le, S. B. (Ekstern), Markussen, S. (Ekstern), Skiadas, I. V. (Intern), Gavala, H. N. (Intern)
Pages: 149-161
Publication date: 2017
Main Research Area: Technical/natural sciences
Controlling sewer systems – a critical review based on systems in three EU cities

The term Real Time Control (RTC) is widely used to describe all types of control systems in sewer systems. Today the term covers everything from the simplest to the most advanced types of control systems, making it difficult to communicate about sewer system control in a precise manner, as well as search and find specific types of control systems for comparison. Through a survey of implemented control systems in three EU cities today and with the perspectives of current research within the field of sewer system control, the needs for a new control system design framework is identified. With the basis of existing frameworks for control system design, a new time-scale dependent framework is proposed. We believe this comprehensive time-scale dependent framework can help water utilities to retrofit and design new control solutions and facilitate knowledge sharing about existing designs.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Systems, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, HOFOR A/S, Biofos A/S
Authors: Mollerup, A. L. (Ekstern), Mikkelsen, P. S. (Intern), Thornberg, D. (Ekstern), Sin, G. (Intern)
Number of pages: 8
Pages: 435-442
Publication date: 2017
Main Research Area: Technical/natural sciences

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Journal: Urban Water Journal
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Issue number: 4
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.689 SNIP 1.192 CiteScore 1.87
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.583 SNIP 1.141 CiteScore 1.42
Conversion of furan derivatives for preparation of biofuels over Ni-Cu/C catalyst

Conversions of furfural and 5-hydroxymethylfurfural as model components in bio-oil were investigated over Ni-Cu/C catalyst with formic acid as hydrogen donor in isopropanol solvent to produce biofuels. The effects of reaction temperature, feed ratio, and reaction time were studied. A high yield of 2-methylfuran up to 91 mol% was obtained from furfural in 8 h at 200°C, and under same conditions 80 mol% yield of 2,5-dimethylfuran could also be obtained from 5-hydroxymethylfurfural in 6 h. The results verified the catalyst performance and the availability of the reaction conditions for producing biofuels from furan derivatives.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Chinese Academy of Sciences
Authors: Fu, Z. (Ekstern), Wang, Z. (Ekstern), Lin, W. (Intern), Song, W. (Ekstern)
Number of pages: 6
Pages: 1176-1181
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Sources. Part A. Recovery, Utilization, and Environmental Effects
Volume: 39
Issue number: 11
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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BFI (2016): BFI-level 1
Corrigendum to “Comparison of Different Strategies for Selection/Adaptation of Mixed Microbial Cultures Able to Ferment Crude Glycerol Derived from Second-Generation Biodiesel”
[This corrects the article DOI: 10.1155/2015/932934.]

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, SINTEF
Authors: Varrone, C. (Intern), Heggeset, T. M. B. (Ekstern), Le, S. B. (Ekstern), Haugen, T. (Ekstern), Markussen, S. (Ekstern), Skiadas, I. V. (Intern), Gavala, H. N. (Intern)
Number of pages: 1
Pages: 7602495
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.32 SJR 0.843 SNIP 0.875
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.822 SNIP 0.756 CiteScore 1.77
Cost competitive "soft sensor" for determining product recovery in industrial methanol

The measurement of ratio of product recovery in industrial methanol distillation is of high economic importance and represent a key performance index (KPI) of the distillation unit. In current operations, the product recovery of many industrial distillation units are not actively monitored, instead back calculated from daily production reports. The active monitoring of product recovery can be a costly affair as it requires expensive gas chromatographs and accurate feed mass flow measuring devices to be installed. Historically, this has been one of the key reasons for not actively monitoring product recovery. In this work a novel, simple and economical method based on density and flow rate measurements to calculate the product recovery of industrial methanol distillation columns has been developed. This method has been validated against plant measurements as well as a validated process simulation. Step and disturbance tests carried out suggest the proposed method is able to accurately estimate the product recovery within the plant operational envelope, but lacks the ability to capture the process dynamics during process changes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, S&D Consulting LLC, Technical University of Applied Sciences, Nürnberg, University of Auckland
Authors: S.B.A. Udugama, I. (Intern), Mansouri, S. S. (Intern), Huusom, J. K. (Intern), Taube, M. A. (Ekstern), Maidl, A. (Ekstern), Young, B. (Ekstern)
Pages: 23-28
Publication date: 2017

Host publication information
Crude fucoidan content in two North Atlantic kelp species, Saccharina latissima and Laminaria digitata - seasonal variation and impact of environmental factors

Fucoidans are sulphated fucose-rich polysaccharides predominantly found in the cell walls of brown algae. The bioactive properties of fucoidans attract increasing interest from the medico-pharmaceutical industries and may drive an increase in demand of brown algae biomass. In nature, the biochemical composition of brown algae displays a seasonal fluctuation driven by environmental factors and endogenous rhythms. To cultivate and harvest kelps with high yields of fucoidans, knowledge is needed on seasonal variation and impact of environmental conditions on the fucoidan content of brown algae. The relations between the fucoidan content and key environmental factors (irradiance, nutrient availability, salinity and exposure) were examined by sampling natural populations of the common North Atlantic kelps, Saccharina latissima and Laminaria digitata, over a full year at Hanstholm in the North Sea and Aarhus in the Kattegat. In addition, laboratory experiments were carried out isolating the effects of the single factors. The results demonstrated that (1) seasonal variation alters the fucoidan content by a factor of 2â€“2.6; (2) interspecific differences exist in the concentrations of crude fucoidan (% of dry matter): L. digitata (11%) > S. latissima (6%); and (3) the effects of single environmental factors were not consistent between species or between different conspecific populations. The ambiguous response to single environmental factors complicates prospective directions for manipulating an increased content of fucoidan in a cultivation scenario and emphasizes the need for knowledge on performance of local kelp ecotypes.
Crystallinity of polyethylene in uni-axial extensional flow

Flow history of polymer melts in processing greatly influences the crystallinity and hence the solid properties of the final material. A wide range of polymer processes involve extensional flows e.g. fiber spinning, blow moulding etc. However, due to instrumental difficulties, experimental studies on polymer crystallization in controlled uniaxial extension are quite rare compared to studies of crystallization in shear. Inherently uniaxial extensional flows are strong and simple relative to shear flows, in the sense that chain stretch is easily obtained and that the molecules experience no tumbling, hence much can be learned from studying polymers in extension. Recent advances in filament stretching rheometry now enable the performance of controlled uniaxial stretching of polymeric liquids even to high Hencky strains [1]. In addition the instrument allows for quenching at specific strains such that crystallization from a stretched state can take place. In this work we explore this feature in the attempt to link the nonlinear extensional rheology to the final morphology. We investigate polyethylenes (PE) of various chain architectures and observe that, even for complex architectures like long chain branched PE, the final morphology is determined by the stress at quench. This can be explained by realizing that nonlinearity in stress arises from changes in molecular configuration such as chain stretch. Hence the nonlinear stress response reflects the molecular configuration during stretching determining the final morphology [2].

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, California Institute of Technology, University of Copenhagen, University of Nottingham
Data Requirements and Modeling for Gas Hydrate-Related Mixtures and a Comparison of Two Association Models

The association theory-based advanced thermodynamic models have gained more and more attention and applications in many industries. The cubic plus association (CPA) and the simplified perturbed chain statistical associating fluid theory (sPC-SAFT) equations of state (EOS) are two of the most widely used association models in the chemical and petroleum industries. The CPA model is extensively used in flow assurance, in which the gas hydrate formation is one of the central topics. Experimental data play a vital role in validating models and obtaining model parameters. In this work, we will compare the performance of the CPA and sPC-SAFT EOS for modeling the fluid-phase equilibria of gas hydrate-related systems and will try to explore how the models can help in suggesting experimental measurements. These systems contain water, hydrocarbon (alkane or aromatic), and either methanol or monoethylene glycol. It is well known that the determination of SAFT-type model parameters for associating fluids remains a challenge because there are at least five pure-component parameters for these compounds and there is no property combination found to be enough to ensure the best parameter set. Therefore, in this work two parameter sets have been chosen for the sPC-SAFT EOS for a fair comparison. The comparisons are made for pure fluid properties, vapor liquid-equilibria, and liquid liquid equilibria of binary and ternary mixtures as well as vapor liquid liquid equilibria of quaternary mixtures. The results show, from an overall point of view, that these two models have equally good performance, and the two parameter sets with the sPC-SAFT EOS are also comparable, especially for the vapor liquid-equilibria systems. Moreover, the modeling results suggest that some data are less reliable than others, which indicates the need for more measurements to further validate the models, especially for multicomponent systems.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Centre for oil and gas – DTU, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, KT Consortium, Technical University of Denmark
Authors: Liang, X. (Intern), Aloupis, G. (Ekstern), Kontogeorgis, G. M. (Intern)
Pages: 2592-2605
Publication date: 2017
Main Research Area: Technical/natural sciences

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Journal: Journal of Chemical and Engineering Data
Volume: 62
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Data Validation and Modelling of Thermodynamic Properties of Systems with Active Pharmaceutical Ingredients (APIs) in Complex Media for Skin Absorption Processes

This study presents methods for prediction of thermodynamic properties required in development of models for drug skin permeation processes, such as drug solubilities and partition coefficients. For evaluation of these properties, ab initio models such as COSMO-SAC can assist in providing a thermodynamically consistent framework. Recently, a model based on fluctuation theory (FST) of solutions for solid- and liquid-liquid equilibria data correlation has been developed. With a well-established methodology for generating reliable initial parameters used in parameter estimation, this model provides a simple framework for correlation and evaluation of existing data.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Ruszczynski, L. (Intern), Zubov, A. (Intern), Sin, G. (Intern), Abildskov, J. (Ekstern)
Pages: 247-252
Publication date: 2017

Host publication information
Deactivation of SCR catalysts by potassium: A study of potential alkali barrier materials

The use of coatings in order to protect vanadia based SCR catalysts against potassium poisoning has been studied by lab- and pilot-scale experiments. Three-layer pellets, consisting of a layer of a potential coating material situated between layers of fresh and potassium poisoned SCR catalyst, were used to test the ability of the barrier layer to block the diffusion of potassium across the pellet. Of MgO, sepiolite and Hollandite manganese oxide, MgO was the most effective potassium barrier, and no potassium was detected in the MgO layer upon exposure to SCR conditions for 7 days. Two monoliths have been exposed to KCl aerosols at 350 °C in a pilot-scale setup for about 1000 hours. A 3 wt.% V₂O₅-7 wt.% WO₃ /TiO₂ reference catalyst deactivated with an average rate of 0.91 %/day, and SEM-EDS analysis showed complete potassium penetration of the catalyst wall. A similar monolith coated with 8.06 wt.% MgO deactivated with a rate of only 0.24 %/day, relative to the fresh activity of the uncoated reference. The initial observed activity of the coated catalyst was, however, only 58 % of that of the reference, likely due to increased transport limitations and loss of active material during the coating process. Potassium had to some extent penetrated the MgO coat, and SEM analysis revealed it to be rather thick and fragile. Despite these observations, the coating did protect the SCR catalyst against potassium poisoning to some degree, leaving promise of further optimization.
Degradation patterns of silicone-based dielectric elastomers in electrical fields
Silicone elastomers have been heavily investigated as candidates for the flexible insulator material in dielectric elastomer transducers and are as such almost ideal candidates because of their inherent softness and compliance. However, silicone elastomers suffer from low dielectric permittivity. This shortcoming has been attempted optimized through different approaches during recent years. Material optimization with the sole purpose of increasing the dielectric permittivity may lead to the introduction of problematic phenomena such as premature electrical breakdown due to high leakage currents of the thin elastomer film. Within this work, electrical breakdown phenomena of various types of permittivity-enhanced silicone elastomers are investigated. Results showed that different types of polymer backbone chemistries lead to differences in electrical breakdown patterns, which were revealed through SEM imaging. This may pave the way towards a better understanding of electrical breakdown mechanisms of dielectric elastomers and potentially lead to materials with increased electrical breakdown strengths.
**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Swiss Federal Institute of Technology, Foundation for Research and Technology-Hellas

Authors: Scherz, L. F. (Ekstern), Costanzo, S. (Ekstern), Huang, Q. (Intern), Schlutter, A. D. (Ekstern), Vlassopoulos, D. (Ekstern)

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**Publication information**

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.76 SJR 2.557 SNIP 1.507
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.407 SNIP 1.638 CiteScore 5.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.534 SNIP 1.721 CiteScore 5.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.576 SNIP 1.754 CiteScore 6.09
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.779 SNIP 1.58 CiteScore 5.35
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.556 SNIP 1.593 CiteScore 5.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.51 SNIP 1.51
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.962 SNIP 1.533
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.819 SNIP 1.54
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.102 SNIP 1.613
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.987 SNIP 1.714
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.579 SNIP 1.654
Density and Compressibility of Multicomponent n-Alkane Mixtures up to 463 K and 140 MPa

Density measurements of two ternary alkane mixtures (methane/n-butane/n-decane and methane/n-butane/n-dodecane) and two multicomponent mixtures composed of methane/n-butane/n-octane/n-dodecane/n-hexadecane/n-eicosane were performed in the temperature range from (278.15 to 463.15) K and pressures up to 140 MPa. The isothermal compressibility values of these mixtures were obtained by differentiation from a Tait-type fitting of experimental densities as a function of temperature and pressure. Excess volume of the studied mixtures was also determined. Four different equations of state, that is, Soave–Redlich–Kwong (SRK), Peng–Robinson (PR), Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT), and Soave-Benedict-Webb-Rubin (Soave-BWR) were used for predicting the experimental density values as well as the excess volumes.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Technical University of Denmark
Authors: Regueira, T. (Intern), Glykioti, M. (Ekstern), Stenby, E. H. (Intern), Yan, W. (Intern)
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Deposit Shedding in Biomass-Fired Boilers: Shear Adhesion Strength Measurements

Ash deposition on boiler surfaces is a major problem encountered in biomass combustion. Timely removal of ash deposits is essential for optimal boiler operation. In order to improve the understanding of deposit shedding in boilers, this study investigates the adhesion strength of biomass ash from full-scale boilers, as well as model fly ash deposits containing KCl, K_2SO_4, CaO, CaSO_4, SiO_2, K_2CO_3, Fe_2O_3, K_2Si_4O_9, and KOH. Artificial biomass ash deposits were prepared on superheater tubes and sintered in an oven with temperatures ranging from 500 to 1000 °C. Subsequently, the deposits were sheared off by an electrically controlled arm, and the corresponding adhesion strength was measured. The effect of sintering temperature, sintering time, deposit composition, thermal shocks on the deposit, and steel type was investigated. The results reveal that the adhesion strength of ash deposits is dependent on two factors: ash melt fraction, and corrosion occurring at the deposit–tube interface. Adhesion strength increases with increasing sintering temperature, sharply increasing at the ash deformation temperature. However, sintering time, as well as the type of steel used, does not have a significant effect under the investigated conditions. Addition of compounds which increase the melt fraction of the ash deposit, typically by forming a eutectic system, increases the adhesion strength, whereas addition of inert compounds with a high melting point decreases the adhesion strength. Furthermore, the study indicated that sulfation of ash deposits leads to an increase in adhesion strength, while cooling down the deposits after sintering decreases the adhesion strength. Finally, it was observed that adhesion strength data follow a log-normal distribution.
Design and simulation of rate-based CO2 capture processes using carbonic anhydrase (CA) applied to biogas

Today the mix of the energy sector is changing from reduction of CO2 emission from fossil fueled power industry into a general focus on renewable industry which is emitting less greenhouse gases. Renewable fuels like biomass for electricity production or biogas for bio-methane production have a potential to create negative emissions using bio-energy carbon capture and storage (BECCS).

All sectors are still in the need for applying more sustainable carbon capture and storage (CCS) technologies which result in lower energy consumption while reducing the impact on the environment. Recently several promoters have been developed for solvent based technologies, but there is still a need to develop new approaches which can potentially reduce energy consumption even further. Solvents typically used for CCS have the tendency to form carbamate. They are characterized by the speed at which they react with CO2. Advantageous kinetics results in smaller equipment size. But this is not the only benefit.

In this study we deliberately apply a slow reacting solvent, MDEA (methyldiethanolamine). It is in the category of noncarbamate forming tertiary amines, for the same reason it binds less hard to CO2. The advantage is a noticeably lower regeneration energy compared to primary and secondary amines. As a result the cost for stripping is significantly lower. Reactivated slow tertiary amines are applied in this study with the aim of reducing energy consumption. This is achieved by using carbonic anhydrase (CA) enzymes as additives in the slow solvent. The aim of this work is to develop a rate-based model for tertiary MDEA mixed with various amounts of CA. The results show that the properties for biogas are significantly different compared to air and may need to be treated accordingly accurate. This work proves that the typical mass transfer resistance observed in the biogas gas phase is low compared to the resistance in the liquid phase. The consequence is a reduced requirement for accurate properties for the biogas and the biogas can easily be modelled as being similar to air. In this work we create a calculation engine which is capable of BECCS, thereby enabling prevention of CO2 emissions from renewable technologies giving a potential for zero-emission scenarios which can help to reach the new low emission CO2 target set up by COP21

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Scopus rating (2014): SJR 0.433 SNIP 0.81 CiteScore 1.09
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Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
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Design, economics and parameter uncertainty in dynamic operation of post-combustion CO₂ capture using piperazine (PZ) and MEA

Post-combustion capture is a promising solution to mitigate the anthropogenic CO₂ emission rate and reduce global warming. However, to make it economically attractive, the techno-economic performance of this process needs to be improved. This includes steady-state but also dynamic operation of the plant. Flexibility is particularly crucial from an economic and operational point of view since plants must balance the power production and the electricity demand on a daily basis.

This work shows the impact of design decisions and uncertainties on the dynamic operation and economics of a CO₂ capture plant using piperazine (PZ), compared to the benchmark MEA solvent. This is exemplified through dynamic model calculations. The results show that the capacity of the buffer tank is a key parameter for the flexibility of the plant. A small tank corresponds to lower capital cost but it leads to increased operation cost and also to flexibility/controllability issues. Both, the PZ and MEA plants present inverse response for small tanks. These plants are challenging to control.
Designing a Surrogate Fuel for Gas-to-Liquid Derived Diesel

Synthetic diesel fuel produced from natural gas via gas-to-liquid (GTL) technology is referred to as ultraclean fuel but is still challenged for full certification as diesel fuel. GTL diesel lacks certain hydrocarbons and chemical constituents, which although are benign to the environment, result in a trade-off in performance when used in a diesel engine. To boost GTL diesel physicochemical properties and thereby enable its use in conventional diesel engines, GTL diesel needs improvement. This can be achieved by mixing suitable additives to the GTL diesel and through the development of surrogate fuels that have fewer components. Screening of thousands of additives is a tedious task and can be done efficiently via computer based modeling to quickly and reliably identify a small number of promising candidates. These models are used to guide the formulation of five surrogates and predict their physicochemical properties. These surrogates are further verified using rigorous mathematical tools as well as through advanced experimental techniques. An optimal surrogate MI-5 is identified, which closely mimics GTL diesel-conventional diesel blends in terms of its physicochemical properties. An engine study for the surrogate is also performed to understand the effect of physicochemical properties on combustion as well as the emission behavior of the fuel. MI-5 exhibited an optimal torque at higher load conditions. A reduction of 11.26% NOx emission for MI-5 is observed when compared to conventional fuel. At higher loads, diesel fuel surpasses the total hydrocarbon (THC) emissions for both the surrogate and the GTL fuel. No significant variation in CO and CO2 emissions for MI-5, GTL diesel and conventional diesel is observed. Analysis of combustion as well as emission behavior of the fuels helps to understand the role of physicochemical properties on the performance of the fuel.
Design of a gas-inducing impeller using Computational Fluid Dynamics

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Technical University of Denmark, BIO-AQUA
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Design of Continuous Crystallizers for Production of Active Pharmaceutical Ingredients
The production of Active Pharmaceutical Ingredients (APIs) is conducted primarily in batch processes. This manufacturing approach is reinforced by a patent-driven business model and the need to minimize the process development times for newly patented drugs. However, the regulatory and business environments are now changing. The increasing costs of drug development, combined with the strict regulations and the competition from generic manufacturers, have pushed pharmaceutical companies to seek cheaper and more sustainable production methods.
Transition from batch to Continuous Pharmaceutical Manufacturing (CPM) could lead to significant reductions in the production costs and an improved consistency of the product quality. As a result, development of such processes has received a significant interest in the past decade. To be able to compete in a patent-driven industry with relatively small annual production rates, CPM should be conducted in versatile units that offer short process development times and can be used for production of different compounds.
This PhD project deals with the development of novel crystallizer configurations and process design methods oriented to
the crystallization of APIs with strict requirements for the control of crystal size and shape. The project includes the development of methods for the early assessment of crystal quality and the evaluation of techniques for improved control of crystallization kinetics in continuous systems.

In the first block of the PhD, a two-stage continuous Mixed Suspension Mixed Product Removal (MSMPR) crystallization setup was designed for the production of an API presenting elongated crystals. A step by step characterization was applied based on image analysis of the crystallization magma, from which the effects of process conditions on crystal size and shape were evaluated. Crystal breakage was found to be highly selective for a single crystal plane, leading to a significant broadening of the crystal shape distribution. This behavior was consistent with the observations in full-scale batch production, where the crystallization product is subject to significant mechanical stress in downstream processing.

The attainable regions for the MSMPR cascade were obtained through a population balance model that is based on the real crystal dimensions obtained from image analysis. Finally, the crystallizer was optimized for a crystal dimension that is consistent through a moderate degree of crystal breakage during downstream processing.

The second block of the PhD involves a fundamental study of the effect of gas dispersion on crystal nucleation kinetics. It is frequently stated in the literature that the presence of an inert gas in a crystallizer can have an impact on crystallization kinetics, either via an improved mass transfer in the crystallizing suspension or by promoting heterogeneous nucleation. These statements are supported by a variety of studies in batch mode. However, the mechanisms are not yet fully understood. In this thesis, the effect of injecting a saturated gas on batch crystallization kinetics has been evaluated from experimental induction times. Combining induction time statistics with a detection method based on sample turbidity, the average time for crystal formation is separated from a detection delay that is a function of the rates of secondary nucleation and crystal growth. Results show a consistent 5-fold reduction in the detection delay for two model systems, and an effect on primary nucleation that is sensitive to the gas injection rate and the studied solute. These results indicate that the induction time reductions frequently reported in the literature could actually be a consequence of a faster crystallization rate after the first nuclei is formed. The mechanism behind these observations is presumably related to a significant improvement in the mixing pattern and intensity.

A novel continuous crystallizer design based on self-induced gas dispersion is presented and evaluated in the last block of the PhD. The objective was to evaluate if gas dispersion could be used to generate smaller crystals in an MSMPR crystallizer, as well as to further develop the understanding of the effect of a moving gas on secondary nucleation and crystal growth. The effect of gas dispersion on crystallization yield and crystal size distribution has been evaluated for a configuration that would be expected in an implemented process, and for operating conditions that are already optimized for the generation of small crystals. Results show that, in contrast with the observations in batch crystallizers, the effect of gas dispersion on a well-mixed MSMPR crystallizer is very limited. Further studies on the effect of impeller speed revealed that crystallization kinetics are not sensitive to variations in the mixing intensity for conditions that meet the requirements for homogeneous three-phase mixing. Results from this study further support the hypothesis that a moving gas phase is an alternative to promote different mixing conditions and demonstrate the limited applicability of this technique in a continuous MSMPR crystallizer.

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Design of Trypanosoma rangeli sialidase variants with improved trans-sialidase activity
A sialidase (EC 3.2.1.18) from the non-pathogenic Trypanosoma rangeli, TrSA, has been shown to exert trans-sialidase activity after mutation of five specific amino acids in the active site (M96V, A98P, S120Y, G249Y, Q284P) to form the so-called TrSASmut enzyme. By computational and hypothesis driven approaches additional mutations enhancing the trans-sialidase activity have been suggested. In the present work, we made a systematic combination of these mutations leading to seven new variants of the T. rangeli sialidase, having 6-16 targeted amino acid mutations. The resulting enzyme variants were analyzed via kinetics for their ability to carry out trans-sialidase reaction using CGMP and D-lactose as substrates. The sialidase variants with 15 and 16 mutations, respectively, exhibited significantly improved trans-sialidase
activity for D-lactose sialylation. Our results corroborate, that computational studies of trans-glycosylation can be a valuable input in the design of novel trans-glycosidases, but also highlight the importance of experimental validation in order to assess the performance. In conclusion, two of the seven mutants displayed a dramatic switch in specificity from hydrolysis towards trans-sialylation and constitute the most potent trans-sialidase mutants of TrSA described in literature to date.

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Scopus rating (2016): CiteScore 3.11 SJR 1.201 SNIP 1.092
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2010): SJR 2.631 SNIP 1.161
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 2.473 SNIP 0.985
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Web of Science (2006): Indexed yes
Determination of Zinc Sulfide Solubility to High Temperatures

A new experimental set-up and methodology for the measurement of ZnS solubility in aqueous solutions at 40, 60 and 80 °C (atmospheric pressure) is presented. The methodology implemented includes the preparation of the samples in a reduced oxygen atmosphere, particle size analysis of ZnS, quality control of the analytical technique and evaluation of equilibration time. ZnS solubility analyses were run for prolonged times (up to 11 days) to ensure that equilibrium conditions were met. The equilibration time was explored at three temperatures (40, 60 and 80 °C) observing small variations in the time required to reach the solid-liquid equilibrium at each temperature. Equilibrium was reached within 72 h. The concentration of zinc and of total sulfur were determined using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). The experimental solubility data show an exponential dependency of the solubility with respect to temperature. An increase of 40 °C results in an increase of roughly 12 times for the solubility of ZnS.

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemistry
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.493 SNIP 0.896 CiteScore 1.28
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.485 SNIP 0.805 CiteScore 1.25
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.505 SNIP 0.815 CiteScore 1.25
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.439 SNIP 0.838 CiteScore 1.31
Development of a Bacterial Biosensor for Rapid Screening of Yeast p-Coumaric Acid Production

Transcription factor-based biosensors are used to identify producer strains, a critical bottleneck in cell factory engineering. Here, we address two challenges with this methodology: transplantation of heterologous transcriptional regulators into new hosts to generate functional biosensors and biosensing of the extracellular product concentration that accurately reflects the effective cell factory production capacity. We describe the effects of different translation initiation rates on the dynamic range of a p-coumaric acid biosensor based on the Bacillus subtilis transcriptional repressor PadR by varying its ribosomal binding site. Furthermore, we demonstrate the functionality of this p-coumaric acid biosensor in Escherichia coli and Corynebacterium glutamicum. Finally, we encapsulate yeast p-coumaric acid-producing cells with E. coli-biosensing cells in picoliter droplets and, in a microfluidic device, rapidly sort droplets containing yeast cells producing high amounts of extracellular p-coumaric acid using the fluorescent E. coli biosensor signal. As additional biosensors become available, such approaches will find broad applications for screening of an extracellular product.

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Organisations: Novo Nordisk Foundation Center for Biosustainability, Bacterial Synthetic Biology, Department of Biotechnology and Biomedicine, Network Engineering of Eukaryotic Cell factories, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, KTH - Royal Institute of Technology, Research Centre Julich (FZJ)
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Development of an Intensified Reactive Distillation Process for the Synthesis of Dioxolane Products

A methodology for process intensification that reduces the number of pieces of equipment as part of the design of a chemical process is presented. The method is based on three stages, the first one to detect feasible process alternatives, the second one to identify intensification opportunities, and in the third one phenomena building blocks are used to develop the best intensified process. The methodology is applied for the intensification of an aldolization process for the synthesis of dioxolane products, based on reacting ethylene glycol and 1,2-butanediol with acetaldehyde to produce 2-methyl,1,3-dioxolane (2MD) and 4-ethyl,2-methyl,1,3-dioxolane (4EMD). It is shown how a base flowsheet is effectively converted into an intensified reactive distillation process with the application of the intensification methodology.

General information
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Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Instituto Tecnológico de Celaya
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Development of a thiol-ene based screening platform for enzyme immobilization demonstrated using horseradish peroxidase

Efficient immobilization of enzymes on support surfaces requires an exact match between the surface chemistry and the specific enzyme. A successful match would normally be identified through time consuming screening of conventional resins in multiple experiments testing individual immobilization strategies. In this study we present a versatile strategy that largely expands the number of possible surface functionalities for enzyme immobilization in a single, generic platform. The combination of many individual surface chemistries and thus immobilization methods in one modular system permits faster and more efficient screening, which we believe will result in a higher chance of discovery of optimal surface/enzyme interactions. The proposed system consists of a thiol-functional microplate prepared through fast photochemical curing of an off-stoichiometric thiol-ene (OSTE) mixture. Surface functionalization by thiol-ene chemistry (TEC) resulted in the formation of a functional monolayer in each well, whereas, polymer surface grafts were introduced through surface chain transfer free radical polymerization (SCT-FRP). Enzyme immobilization on the modified surfaces was evaluated by using a rhodamine labeled horseradish peroxidase (Rho-HRP) as a model enzyme, and the amount of immobilized enzyme was qualitatively assessed by fluorescence intensity (FI) measurements. Subsequently, Rho-HRP activity was measured directly on the surface. The broad range of utilized surface chemistries permits direct correlation of enzymatic activity to
the surface functionality and improves the determination of promising enzyme-surface candidates. The results underline
the high potential of this system as a screening platform for synergistic immobilization of enzymes onto thiol-ene polymer
surfaces. This article is protected by copyright. All rights reserved.

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for BioProcess
Engineering, CAPEC-PROCESS
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Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.727 SNIP 0.825 CiteScore 2.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.764 SNIP 0.847 CiteScore 2.16
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.84 SNIP 0.868 CiteScore 2.35
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.918 SNIP 0.956 CiteScore 2.4
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.988 SNIP 0.947
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.965 SNIP 1.047
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.887 SNIP 0.992
Scopus rating (2007): SJR 1.011 SNIP 1.093
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.973 SNIP 1.108
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.905 SNIP 1.029
Web of Science (2005): Indexed yes
Development of highly efficient solid oxide electrolyzer cell systems

Solid oxide electrolyzer cells (SOEC) are electrochemical devices capable of converting H₂O or CO₂ to H₂ and CO, respectively. In this thesis, the possibility of production of CO with SOECs are investigated, since it is currently of commercial interest, but could also play a major role in the future energy system.

The overall objective of the thesis was to investigate the limits for the allowed CO concentration during electrolysis of CO₂ in SOECs and how the limit could be increased. A high CO concentration is desired because it lowers the strain on the separation unit and amount of recycle, when SOECs are used in systems like Haldor Topsoe A/S’s “eCOs”. In this way, the overall efficiency of SOEC systems are increased. The CO concentration was limited by carbon formation via the Boudouard reaction, a non-uniform flow in the fuel channels over the fuel electrode, and the diffusion in the fuel electrode.

The thesis has focused on obtaining knowledge on the limiting causes, through both experimental work and modeling. The formation of carbon leads to delamination of the cell layers and ultimately destroys the cells. It was found that the carbon formation was hindered, when the Boudouard reaction was thermodynamically unfavored. From thermo-gravimetry analyzer experiments, the thermodynamics for the equilibrium for the Boudouard reaction was obtained for Ni-YSZ material used in SOECs.

It is important that the flow distribution in the cell is as uniform as possible, since non-uniformities will lead to regions with low CO concentration. The flow distribution in the fuel channels over the fuel electrode was investigated with computational fluid dynamics (CFD) modeling. The flow was optimized by changing the cell inlet geometry and an increase in the flow uniformity was observed. The impact on the allowed average (exit) CO concentration was quite high (from 22 to 32 %).

The effective diffusion in the fuel electrode was investigated with a Wicke-Kallenbach set up. Combined with measurements of the thickness, porosity and pore size, the tortuosity of the material was calculated. This made it possible to implement the diffusion limitation in an in-house 3d stack model and evaluate the impact of diffusion limitations (only included in the confidential version of the thesis). The local CO concentration is limited by the thermodynamics for the Boudouard reaction. The diffusion cause an increase in the CO concentration at the reaction sites, compared to the channel, and diffusion therefore limits the allowed CO concentration in the fuel channel. The diffusion was found to be low, resulting in large concentration gradients between the channel and reaction sites. This mean that the allowed CO concentration in the fuel channel is very limited by diffusion.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS
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Development of in-situ product removal strategies in biocatalysis applying scaled-down unit operations
An experimental platform based on scaled-down unit operations combined in a plug-and-play manner enables easy and highly flexible testing of advanced biocatalytic process options such as in-situ product removal (ISPR) process strategies. In such a platform it is possible to compartmentalize different process steps while operating it as a combined system, giving the possibility to test and characterize the performance of novel process concepts and biocatalysts with minimal influence of inhibitory products. Here the capabilities of performing process development by applying scaled-down unit operations are highlighted through a case study investigating the asymmetric synthesis of 1-methyl-3-phenylpropylamine (MPPA) using ω-transaminase, an enzyme in the sub-family of amino transferases (ATAs). An on-line HPLC system was applied to avoid manual sample handling and to semi-automatically characterize ω-transaminases in a scaled-down packed-bed reactor (PBR) module, showing MPPA as a strong inhibitor. To overcome the inhibition, a two-step liquid-liquid extraction (LLE) ISPR concept was tested using scaled-down unit operations combined in a plug-and-play manner. Through the tested ISPR concept, it was possible to continuously feed the main substrate benzylacetone (BA) and extract the main product MPPA throughout the reaction, thereby overcoming the challenges of low substrate solubility and product inhibition. The tested ISPR concept achieved a product concentration of $26.5 \text{gMPPA·L}^{-1}$, a purity up to $70\% \text{gMPPA·L}^{-1}$ and a recovery in the range of 80% mol·mol$^{-1}$ of MPPA in 20 hours, with the possibility to increase the concentration, purity and recovery further. This article is protected by copyright. All rights reserved

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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.589 SNIP 1.401 CiteScore 4.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.621 SNIP 1.425 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.639 SNIP 1.366 CiteScore 4.04
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Web of Science (2012): Indexed yes
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Development of New Diesel Oxidation and NH$_3$ Slip Catalysts

Diesel engines used in the transport sector and for other heavy machinery form pollutants during the combustion process. Emission of these pollutants into the atmosphere has harmful consequences on human health and the environment. In order to mitigate these harmful effects, regulations have been imposed by environmental protection agencies on the most significant pollutants, including CO, hydrocarbons, NO, and particulate matter. To reduce emissions to the levels specified by the recent Euro VI regulations, it is necessary to apply catalytic exhaust gas aftertreatment systems.

A modern diesel exhaust aftertreatment system commonly consists of a Pt-based diesel oxidation catalyst (DOC) to oxidize CO and unburnt hydrocarbons to CO$_2$ and H$_2$O, and oxidize NO to NO$_2$. This is followed by the diesel particulate filter (DPF), which entraps particulate matter from the exhaust gas. A solution of urea is injected after the DPF to supply NH$_3$ for the selective catalytic reduction (SCR) of NO over an NH$_3$-SCR catalyst. A mixture of NO and some NO$_2$ evokes the fast SCR reaction, which increases NO$_x$ reduction. Emissions of NO$_x$ can be further decreased by dosing a stoichiometric excess of NH$_3$. However, NH$_3$ is also a regulated pollutant and it is therefore necessary to include an ammonia slip catalyst (ASC) for the selective catalytic oxidation of excess NH$_3$ to N$_2$ and H$_2$O.

The purpose of this research project has been to develop an optimized diesel oxidation catalyst with a low noble metal content and a highly active ammonia slip catalyst with an improved N$_2$ selectivity.

The Pt-based DOC constitutes a significant part of system costs. To effectively utilize the platinum and reduce cost, the influence of Pt particle size on catalytic activity for CO, hydrocarbon, and NO oxidation was studied using 1 wt.% Pt/Al$_2$O$_3$ catalysts with Pt particles diameters between 1.3 and 18.7 nm. The mass based oxidation activity of CO, C$_3$H$_6$, and NO showed an optimal Pt particle size between 2–4 nm for all three reactions. Based on the turnover frequencies and the distribution of surface atoms of Pt particles, the reactions appear to be mainly catalyzed by terrace atoms, which are most abundant between 2–4 nm. The decrease in catalytic activity for large Pt particles can be explained by the diminishing Pt
surface area, while the decrease in activity for small particles is due to the lack of terrace atoms required for catalyzing the oxidation of CO, hydrocarbons, and NO.

The modern ASC is a multi-functional catalyst that combines the high ammonia oxidation (AMOX) activity of a Pt-based catalyst with the capability of an SCR catalyst to reduce formed NOx to N2 using NH3. The high selectivity of the AMOX catalyst towards N2O and NOx at temperatures above 225–250°C, corresponding to a poor N2 selectivity, is counterproductive for the aftertreatment system. By including an SCR catalyst, the N2 selectivity is greatly improved. The AMOX component of the ASC was considered by investigating the catalytic oxidation of NH3 over a series of noble metal catalysts (1 wt.% Pt/Al2O3, 5 wt.% Pt/Al2O3, 5 wt.% Rh/Al2O3, and 5 wt.% Pd/Al2O3). The Pt catalysts were the most active and a series of 1 wt.% Pt/Al2O3 catalysts with varying Pt particle sizes of 1.3–18.7 nm and of ~200 nm was subsequently tested. Large Pt particles of 7.7 nm, 18.7 nm, and ~200 nm were the most active, and Pt particles of ~200 nm also achieved lower yields of N2O and NO2 but with an increase in the total NOx formed. Furthermore, Pt particles of 2–4 nm achieved the greatest NO2/NOx ratios, in line with observations for NO oxidation over 1 wt.% Pt/Al2O3.

A single channel 1D-1D steady state mathematical model of the ammonia slip catalyst was further developed and validated in order to improve system understanding and reduce experimental efforts. The model includes film diffusion from the gas channel to the washcoat surface, and the diffusion and reaction throughout the washcoat layers of one monolith channel. The kinetic models applied were derived based on activity measurements for 1 wt.% Pt/TiO2-SiO2 (AMOX) and 3.5 wt.%Cu-BEA (SCR). The monolith model was validated against experimental data for NH3 oxidation over four monolithic catalysts: single layer AMOX, single layer SCR, single mixed layer, and dual layer configurations. The model description agrees well with experimental data for NH3 conversion and selectivities to NOx, N2O, and N2. The validated model was used to analyze the performance of the single layer and dual layer ammonia slip catalysts with respect to variations in the following parameters: the intrinsic activity of the AMOX catalyst, the loadings of the AMOX and SCR catalysts, the effective diffusivity of the catalyst layers, the NO oxidation activity of the AMOX catalyst, and the ability of each catalyst to form N2O. For all ASC catalysts, an adequate Pt loading is necessary since it determines the ammonia oxidation activity available. If the Pt loading is sufficient, then the catalyst loadings and effective diffusivity become the key design parameters since these factors determine the effectiveness factor of the catalyst and the magnitude of SCR activity available for NOx reduction. By varying the NO oxidation activity of the AMOX catalyst it is possible to alter the NO2/NOx ratio and evoke the fast SCR reaction, thereby improving NOx reduction, but also increasing N2O selectivity. Addition-ally, excluding N2O formation from either the AMOX or SCR catalyst identified the AMOX catalyst as the main source of N2O formation. Thus, development of an ASC with low N2O yield should focus on the AMOX component. The multi-objective optimization of ten ASC configurations for NH3 oxidation at 300°C was used to study the sensitivity towards the catalyst architecture of the ASC. The resulting Pareto fronts indicate that the optimal catalyst systems with the most potential are those involving mixed layers of AMOX and SCR catalysts, rather than pure layers of AMOX or a top layer of SCR. This is mainly due to the ability of the mixed layers to circumvent N2O formation with the more immediate reduction of NOx with NH3.
Development of novel monoclonal antibodies against starch and ulvan - Implications for antibody production against polysaccharides with limited immunogenicity

Monoclonal antibodies (mAbs) are widely used and powerful research tools, but the generation of mAbs against glycan epitopes is generally more problematic than against proteins. This is especially significant for research on polysaccharide-rich land plants and algae (Viridiplantae). Most antibody production is based on using single antigens, however, there are significant gaps in the current repertoire of mAbs against some glycan targets with low immunogenicity. We approached mAb production in a different way and immunised with a complex mixture of polysaccharides. The multiplexed screening capability of carbohydrate microarrays was then exploited to deconvolute the specificities of individual mAbs. Using this strategy, we generated a set of novel mAbs, including one against starch (INCh1) and one against ulvan (INCh2). These polysaccharides are important storage and structural polymers respectively, but both are generally considered as having limited immunogenicity. INCh1 and INCh2 therefore represent important new molecular probes for Viridiplantae research. Moreover, since the α-(1-4)-glucan epitope recognised by INCh1 is also a component of glycogen, this mAb can also be used in mammalian systems. We describe the detailed characterisation of INCh1 and INCh2, and discuss the potential of a non-directed mass-screening approach for mAb production against some glycan targets.
Diffusion of sulfuric acid in protective organic coatings

Organic protective coatings and linings are widely used to prevent corrosion in industrial processes. However, the permeation of aggressive chemicals through coatings can induce failures. These are described in the literature, but rarely quantified. To measure the diffusion rates of aggressive chemicals through organic coatings, a diffusion cell was designed. The diffusion cell designed is simple, small and suitable for scaling up to a battery of cells. A concentration profile of H₃O⁺ through epoxy coatings was achieved for sulfuric acid aqueous solutions, which can be used to estimate diffusion coefficients of H₃O⁺. Typically, Crank’s time-lag method is used to estimate the diffusion coefficients but more complicated modelling is required for sulfuric acid solutions. Future modelling work is needed to estimate diffusion behavior of sulfuric acid.

General information

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Hempel AS
Authors: Wang, T. (Intern), Møller, V. B. (Intern), Dam-Johansen, K. (Intern), Frankær, S. M. (Ekstern), Kiil, S. (Intern)
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Diffusion of surface-active amphiphiles in silicone-based fouling-release coatings

Amphiphiles (i.e. amphiphilic molecules such as surfactants, block copolymers and similar compounds) are used in small amounts to modify the surface properties of polymeric materials. In silicone fouling-release coatings, PEG-based amphiphiles are added to provide biofouling-resistance. The success of this approach relies on the ability of the amphiphiles to diffuse through the coating film and cover the surface of the coating. A novel method for the measurement of diffusion coefficients of PEG-based amphiphiles of different chemistries in PDMS-based coatings is presented here. The diffusion coefficient of the amphiphiles shows a weak dependency on their molecular weight, although this dependency is much less pronounced than for other rubbery polymeric materials. The biofouling-resistance properties in fouling-release coatings were also studied for these amphiphiles. It was found that the diffusion coefficient does not have any influence on the biofouling-resistance results for the studied compounds. Instead, the chemistry of the hydrophobic block of the amphiphiles is much more significant, with PEG-PDMS block copolymers showing the best properties among the studied compounds.

General information

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Scopus rating (2013): SJR 1.03 SNIP 1.663 CiteScore 2.58
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Scopus rating (2011): SJR 0.884 SNIP 1.606 CiteScore 2.34
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Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 0.983 SNIP 1.537
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Scopus rating (2009): SJR 0.867 SNIP 1.333
Web of Science (2009): Indexed yes
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Scopus rating (2005): SJR 0.928 SNIP 1.168
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.692 SNIP 1.121
Web of Science (2004): Indexed yes
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Scopus rating (2002): SJR 1.037 SNIP 1.312
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Dimerization of Carboxylic Acids: An Equation of State Approach

The association term of the nonrandom hydrogen bonding theory, which is an equation of state model, is extended to describe the dimerization of carboxylic acids in binary mixtures with inert solvents and in systems of two different acids. Subsequently, the model is applied to describe the excess enthalpies and the vapor-liquid equilibrium of relevant binary mixtures containing low molecular weight organic acids. The model sheds light on the interplay of intermolecular interactions through the calculation of the various contributions to the mixing enthalpies, namely from hydrogen bonding and non-hydrogen bonding (dipolar, induced polar or dispersive) interactions. According to model predictions, the acid molecules are so strongly associated that the addition of inert solvents to carboxylic acids with small carbon numbers at ambient temperature does not dramatically alter their degree of association. Consequently, the observed endothermic dissolution process is mainly attributed to the hindering of polar interactions. Furthermore, upon mixing of two carboxylic acids, the rearrangement of hydrogen bonds due to the formation of cross associating species results in an insignificant contribution to the heats of mixing due to the rather constant dimerization enthalpy that is revealed by the available experimental data for low molecular weight compounds.

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Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.92 SNIP 1.251 CiteScore 3.66
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.78 SNIP 1.226 CiteScore 3.62
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.849 SNIP 1.214
Web of Science (2010): Indexed yes
Laccases (EC 1.10.3.2) catalyse removal of an electron and a proton from phenolic hydroxyl groups, including phenolic hydroxyls in lignins, to form phenoxy radicals during reduction of $O_2$. We employed electron paramagnetic resonance spectroscopy (EPR) for real time measurement of such catalytic radical formation activity on three types of lignin (two types of organosolv lignin, and a lignin rich residue from wheat straw hydrolysis) brought about by two different fungal laccases, derived from Trametes versicolor (Tv) and Myceliophthora thermophila (Mt), respectively. Laccase addition to suspensions of the individual lignin samples produced immediate time and enzyme dose dependent increases in intensity in the EPR signal with $g$-values in the range 2.0047–2.0050 allowing a direct quantitative monitoring of the radical formation and thus allowed laccase enzyme kinetics assessment on lignin. The experimental data verified that the laccases acted upon the insoluble lignin substrates in the suspensions. When the action on the lignin substrates of the two laccases were compared on equal enzyme dosage levels (by activity units on syringaldazine) the Mt laccase exerted a significantly faster radical formation than the Tv laccase on all three types of lignin substrates. When comparing the equal laccase dose rates on the three lignin substrates the enzymatic radical formation rate on the wheat straw lignin residue was consistently higher than those of the organosolv lignins. The $pH$-temperature optimum for the radical formation rate in organosolv lignin was determined by response surface methodology to $pH$ 4.8, 33 °C and $pH$ 5.8, 33 °C for the Tv laccase and the Mt laccase, respectively. The results verify direct radical formation action of fungal laccases on lignin without addition of mediators and the EPR methodology provides a new type of enzyme assay of laccases on lignin.
Diversity of microbial carbohydrate-active enzymes in Danish anaerobic digesters fed with wastewater treatment sludge

Improved carbohydrate-active enzymes (CAZymes) are needed to fulfill the goal of producing food, feed, fuel, chemicals, and materials from biomass. Little is known about how the diverse microbial communities in anaerobic digesters (ADs) metabolize carbohydrates or which CAZymes that are present, making the ADs a unique niche to look for CAZymes that can potentiate the enzyme blends currently used in industry.

Enzymatic assays showed that functional CAZymes were secreted into the AD environments in four full-scale mesophilic Danish ADs fed with primary and surplus sludge from municipal wastewater treatment plants. Metagenomes from the ADs were mined for CAZymes with Homology to Peptide Patterns (HotPep). 19,335 CAZymes were identified of which 30% showed 50% or lower identity to known proteins demonstrating that ADs make up a promising pool for discovery of novel CAZymes. A function was assigned to 54% of all CAZymes identified by HotPep. Many different α-glucan-acting CAZymes were identified in the four metagenomes, and the most abundant family was glycoside hydrolase family 13, which contains α-glucan-acting CAZymes. Cellulytic and xylanolytic CAZymes were also abundant in the four metagenomes. The cellulytic enzymes were limited almost to endoglucanases and β-glucosidases, which reflect the large amount of partly degraded cellulose in the sludge. No dockerin domains were identified suggesting that the cellulytic enzymes in the ADs studied operate independently. Of xylanolytic CAZymes, especially xylanases and β-xylosidase, but also a battery of accessory enzymes, were present in the four ADs.

Our findings suggest that the ADs are a good place to look for novel plant biomass degrading and modifying enzymes that can potentiate biological processes and provide basis for production of a range of added-value products from biorefineries.

**General information**

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**Organisations:** Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Aalborg University

**Authors:** Wilkens, C. (Intern), Busk, P. K. (Intern), Pilgaard, B. (Intern), Zhang, W. (Ekstern), Nielsen, K. L. (Ekstern), Nielsen, P. H. (Ekstern), Lange, L. (Intern)

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Drag resistance measurements for newly applied antifouling coatings and welding seams on ship hull surface

Drag resistances of newly applied antifouling coatings and welding seams on ship hull surface have been investigated using a pilot-scale rotary setup. Both conventional biocide-based antifouling (AF) coatings and silicone-based fouling release (FR) coatings have been studied and compared in their newly applied conditions. The effects of water absorption of newly applied antifouling coatings on frictional resistance were measured. A flexible rotor with artificial welding seams on its periphery has been designed and constructed to estimate the influence of welding seams on drag resistance. Both the density of welding seams (number per 5 m ship side) and the height of welding seams had a significant effect on drag resistance.

Driving Force Based Design of Cyclic Distillation

Driving force based design is adopted from conventional continuous distillation to cyclic distillation. This leads to a definition of the operating line representation for the cyclic distillation process. A possible realization of the driving force design is presented, which implies operation with mixed phase feeds. A range of binary test cases, benzene toluene, methanol water, and ethanol water, are evaluated. The advantage of the design approach in cyclic distillation is shown to be analogous to the advantages obtained in conventional continuous distillation, including a minimal utility consumption of the column and likely less sensitivity to feed composition changes.
Dynamic dilution exponent in monodisperse entangled polymer solutions

We study and model the linear viscoelastic properties of several entangled semi-dilute and concentrated solutions of linear chains of different molar masses and at different concentrations dissolved in their oligomers. We discuss the dilution effect of the oligomers on the entangled long chains. In particular, we investigate the influence of both concentration and molar mass on the value of the effective dynamic dilution exponent determined from the level of the storage plateau at low and intermediate frequencies. We show that the experimental results can be quantitatively explained by considering the tension re-equilibration process along the chains, in agreement with van Ruymbeke et al. (Macromol., 2014), i.e. by considering that the real dilution exponent $\alpha$ is always equal to 1, while larger values of the dilution exponent ($1 < \alpha < 1.3$) found experimentally are attributed to the enhanced relaxation of the long chain extremities. Then we discuss the influence of the polymer concentration on the terminal relaxation time of the solutions and how this can be modelled by the enhanced contour length fluctuation process (CR-CLF). We point out that this larger dilution effect is not only a function of concentration but also depends on the molar mass of the chains. While the proposed approach successfully explains the viscoelastic properties of a large number of semi-dilute solutions of polymers in their own oligomers, important discrepancies are found for semi-dilute entangled polymers in small-molecule theta or good solvents. Possible explanations for the differences between these sample sets are proposed, based on the comparison of their viscoelastic behavior.
A dynamic model of pectin extraction is proposed that describes pectin yield, degree of esterification and intrinsic viscosity. The dynamic model is one dimensional in the peel geometry and includes mass transport of pectin by diffusion and reaction kinetics of hydrolysis, degradation and de-esterification. The model takes into account the effects of the process conditions such as temperature and acid concentration on extraction kinetics. It is shown that the model describes pectin bulk solution concentration, degree of esterification and intrinsic viscosity in pilot scale extractions from lime peel at different temperatures (60 °C, 70 °C, 80 °C) and pH (1.5, 2.3, 3.1) values.
Economic Optimizing Control for Single-Cell Protein Production in a U-Loop Reactor

The production of single-cell protein (SCP) in a U-loop reactor by a methanotroph is a cost efficient sustainable alternative to protein from fish meal obtained by over-fishing the oceans. SCP serves as animal feed. In this paper, we present a mathematical model that describes the dynamics of SCP production in a U-loop reactor. We use this model to compute an
optimal start-up trajectory by solution of an economic optimizing optimal control problem. The optimal start-up trajectory is an unstable attractor. The practical implementation of this optimal start-up trajectory can be conducted by a proportional controller for the substrate concentration in the top tank of the U-loop reactor.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Centre for oil and gas – DTU, Technical University of Denmark
Authors: Drejer, A. (Ekstern), Ritschel, T. K. S. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
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**eCPA: An ion-specific approach to parametrization**
Abstract The eCPA equation of state has been shown to be a promising electrolyte model, for which several applications have been demonstrated. The model at its current status is, however, limited by the use of salt-specific parameters for the interactions between salts and water. Having salt-specific parameters limit the applicability to simple systems of ions, as it can only be applied when a common ion is found between the salts in the solution. For more complex systems of multiple ions/salts this may not work well. In this work the main goal is to eliminate this limitation by parametrizing the model with an ion-specific parameter set. The ion-specific parameters are estimated by a simultaneous fitting of parameters for 17 ions, consisting of 10 cations and 7 anions, and with data for 55 salts. The parameters are fitted to osmotic coefficient and mean ionic activity coefficient data in a wide temperature range from 273.15K to above 500K and up to an ionic strength of 6 molal. The parameters are found to yield similar deviations as the salt-specific parameters, however, for a few salts cation-anion interaction parameters were needed in order to obtain reasonable accuracy. The parameters are applied to a series of systems, which include mixed salt osmotic coefficients, solid-liquid equilibrium and vapor-liquid equilibrium of water-methanol-salt, illustrating the applicability of the ion-specific parameters. Modelling of mixed salt osmotic coefficients illustrate that the parameters work well in salt mixtures, while the phase equilibria also illustrate the extension to mixed solvent systems.

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering, KT Consortium
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ISI indexed (2012): ISI indexed yes
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.293 SNIP 2.127
Web of Science (2008): Indexed yes
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Web of Science (2005): Indexed yes
Effect of Air Injection on Nucleation Rates: An Approach from Induction Time Statistics

From disruption of the supersaturated solution to improved mass transfer in the crystallizing suspension, the introduction of a moving gas phase in a crystallizer could lead to improved rates of nucleation and crystal growth. In this work, saturated air has been injected to batch crystallizers to study the effects on formation of the first crystal and subsequent turbidity buildup. To account for the typically large sample-to-sample variation, nucleation rates were evaluated for a large number of replicates using probability distributions of induction times. The slope and the intercept of the distributions were studied independently, allowing the simultaneous determination of the mean induction time and a certain detection delay related to the rate of crystal growth after formation of the first nucleus. When saturated air was injected in aqueous glycine solutions, the average detection delay was reduced from 69 to 13 min, and the mean induction time decreased from 128 to 36 min. The effect on aqueous solutions of l-arginine was less apparent, with a detection delay reduction from 15 to 3 min, and no significant changes on the rate of primary nucleation. These results demonstrate the potential of this technique for reduction in nucleation induction time and improved mass deposition rates in crystallization operations.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), H. Lundbeck A/S, Massachusetts Institute of Technology
Authors: Capellades Mendez, G. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Mealy, M. J. (Ekstern), Christensen, T. V. (Ekstern), Myerson, A. S. (Ekstern)
Number of pages: 8
Pages: 3287-3294
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Crystal Growth & Design
Volume: 17
Issue number: 6
ISSN (Print): 1528-7483
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4 SJR 1.167 SNIP 1.234
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.279 SNIP 1.335 CiteScore 4.48
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.361 SNIP 1.47 CiteScore 4.84
Effect of flue gas composition on deposit induced high temperature corrosion under laboratory conditions mimicking biomass firing. Part I: Exposures in oxidizing and chlorinating atmospheres

In biomass fired power plants, deposition of alkali chlorides on superheaters, as well as the presence of corrosive flue gas species, give rise to fast corrosion of superheaters. In order to understand the corrosion mechanism under this complex condition, the influence of the flue gas composition on high temperature corrosion of an austenitic superheater material under laboratory conditions mimicking biomass firing is investigated in this work. Exposures involving deposit (KCl)-coated and deposit-free austenitic stainless steel (TP347H FG) samples were conducted isothermally at 560 °C for 72 h, under both oxidizing and oxidizing-chlorinating atmospheres, and the resulting corrosion products were comprehensively studied with scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD) techniques. The results show that deposit-free samples suffer grain boundary attack only in an oxidizing-chlorinating atmosphere, otherwise corrosion results in formation of a duplex oxide. Corrosion attack on deposit-coated samples was higher than on deposit-free samples irrespective of the gaseous atmosphere. Specifically, severe volatilization of alloying elements occurred on deposit-coated samples under oxidizing-chlorinating atmosphere due to enhanced impact of KCl and HCl.

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Okoro, S. C. (Intern), Kiamehr, S. (Intern), Montgomery, M. (Intern), Jappe Frandsen, F. (Intern), Pantleon, K. (Intern)
Pages: 499–514
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials and Corrosion
Volume: 68
Effect of flue gas composition on deposit induced high temperature corrosion under laboratory conditions mimicking biomass firing. Part II: Exposures in SO2 containing atmospheres

In biomass fired power plants, the fast corrosion of superheaters is facilitated by the presence of corrosive flue gas species, for example, SO2, which are released during combustion. To understand the role of the gas species on the corrosion process, comparative laboratory exposures of deposit (KCl)-coated and deposit-free austenitic stainless steel (TP 347H FG) samples to gas mixtures containing SO2 was carried out, under conditions relevant to biomass-firing. Exposures were conducted isothermally at 560 °C for 72 h, in oxidizing-sulphidizing and oxidizing-sulphidizing-chlorinating gas mixtures containing 60 ppmv SO2. Scanning electron microscopy (SEM), energy dispersive X-rayspectroscopy (EDS) and X-ray diffraction (XRD) techniques were complementarily applied to characterize the resulting corrosion products. A partially molten K2SO4-layer formed on KCl coated specimens, and corrosion resulted in localized broad pits containing sulphides and oxides. The severe pitting attack was decreased by the presence of HCl in the gas mixture.

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Okoro, S. C. (Intern), Kiamehr, S. (Intern), Montgomery, M. (Intern), Jappe Frandsen, F. (Intern), Pantleon, K. (Intern)
Pages: 515-528
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials and Corrosion
Volume: 68
Issue number: 5
ISSN (Print): 0947-5117
Ratings:
BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.21 SJR 0.526 SNIP 0.741
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.668 SNIP 1.033 CiteScore 1.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.76 SNIP 1.196 CiteScore 1.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.824 SNIP 1.434 CiteScore 1.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.669 SNIP 1.126 CiteScore 1.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.606 SNIP 1.124 CiteScore 1.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Effect of NO2 and water on the catalytic oxidation of soot

The influence of adding NO2 to 10 vol% O2/N2 on non-catalytic soot oxidation and soot oxidation in intimate or loose contact with a catalyst has been investigated. In non-catalytic soot oxidation the oxidation rate is increased significantly at lower temperatures by NO2. For soot oxidation in tight contact with a Co3O4 catalyst a more reactive NO2-containing atmosphere did not change the oxidation profile significantly during temperature programmed oxidation. This is consistent with the expected Mars van Krevelen mechanism, where the rate limiting step is reaction between carbon and lattice oxygen from the oxide, and where the reaction thus has reached the zero order kinetics regime in the gaseous reactant. In loose contact with a catalyst the presence of NO2 causes a pronounced enhancement of the oxidation rate. The rate constants for loose contact soot oxidation in the presence of NO2 exhibited a volcano-curve dependence on the heat of oxygen chemisorption, and among the tested pure metals and oxides Cr2O3 was the most active catalyst. Further improvements were achieved with a FeaCrbOx binary oxide catalyst.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Christensen, J. M. (Intern), Grunwaldt, J. (Intern), Jensen, A. D. (Intern)
Pages: 182-188
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Catalysis B: Environmental
Volume: 205
ISSN (Print): 0926-3373
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2

Original language: English
DOIs: 10.1002/maco.201609174
Publication: Research - peer-review › Journal article – Annual report year: 2016
Effect of Water Clustering on the Activity of Candida antarctica Lipase B in Organic Medium

The effect of initial water activity of MTBE (methyl tert-butyl ether) medium on CALB (Candida antarctica lipase B) catalyzed esterification reaction is investigated using experimental methods and classical molecular dynamics (MD) simulations. The experimental kinetic studies show that the initial reaction rate of CALB-catalyzed esterification reaction between butyric acid and ethanol decreases with increasing initial water activity of the medium. The highest rate of esterification is observed at the lowest water activity studied. MD simulations were performed to gain a molecular insight...
on the effect of initial water activity on the rate of CALB-catalyzed reaction. Our results show that hydration has an insignificant effect on the structure and flexibility of CALB. Rather, it appears that water molecules bind to certain regions ("hot spots") on the CALB surface and form clusters. The size of the water clusters at these hot spot regions gradually increase and expand with increasing water activity. Consequently, the surface area of CALB covered by the water molecules also increases. Specifically, our results indicate that a particular water cluster located close to the active site partially cover the binding pocket of substrate at high water activity. As a consequence, the effective concentration of substrate at the catalytic site decreases. Therefore, the reaction rate slows down with increasing water activity, which correlates well with the observed decrease in the experimentally determined initial reaction rate.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
Authors: Banik, S. D. (Intern), Nordblad, M. (Intern), Woodley, J. M. (Intern), Peters, G. H. (Intern)
Publication date: 2017
Main Research Area: Technical/natural sciences

Electrical breakdown phenomena of dielectric elastomers
Silicone elastomers have been heavily investigated as candidates for dielectric elastomers and are as such almost ideal candidates with their inherent softness and compliance but they suffer from low dielectric permittivity. This shortcoming has been sought optimized by many means during recent years. However, optimization with respect to the dielectric permittivity solely may lead to other problematic phenomena such as premature electrical breakdown. In this work, we investigate the electrical breakdown phenomena of various types of permittivity-enhanced silicone elastomers. Two types of silicone elastomers are investigated and different types of breakdown are discussed. Furthermore the use of voltage stabilizers in silicone-based dielectric elastomers is investigated and discussed.

General information
Electrical breakdown phenomena of dielectric elastomers

Silicone elastomers have been heavily investigated as candidates for dielectric elastomers and are as such almost ideal candidates with their inherent softness and compliance but they suffer from low dielectric permittivity.[1] This shortcoming has been sought optimized by many means during recent years. However, optimization with respect to the dielectric permittivity solely may lead to other problematic phenomena such as premature electrical breakdown. In this work, we focus on the chloro propyl functionalized silicone elastomers prepared in Madsen et al[2] and we investigate the electrical breakdown patterns of two similar chloro propyl functionalized silicone elastomers which break down electrically in a rather different way as well as we compare them to a silicone based reference. Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray Spectroscopy (EDS) are used to evaluate the elastomers after electrical breakdown.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Electron Nanoscopy
Authors: Yu, L. (Intern), Mateiu, R. V. (Intern), Skov, A. L. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at International Conference on Electromechanically Active Polymer (EAP) transducers & artificial muscles, Cartagena, Spain.
Main Research Area: Technical/natural sciences
Electronic versions:
EuroEAP2017_Liyun_Yu_DTU_eaposter_submitted.pdf
Publication: Research - peer-review › Poster – Annual report year: 2017

Electrical breakdown phenomena of dielectric elastomers

Silicone elastomers have been heavily investigated as candidates for dielectric elastomers and are as such almost ideal candidates with their inherent softness and compliance but they suffer from low dielectric permittivity.[1] This shortcoming has been sought optimized by many means during recent years. However, optimization with respect to the dielectric permittivity solely may lead to other problematic phenomena such as premature electrical breakdown.

In this work, we focus on the chloro propyl functionalized silicone elastomers prepared in Madsen et al[2] and we investigate the electrical breakdown patterns of two similar chloro propyl functionalized silicone elastomers which break down electrically in a rather different way as well as we compare them to a silicone based reference. Thermogravimetric analysis (TGA) and scanning electron microscopy (SEM) are used to evaluate the elastomers before and after electrical breakdown. It was shown the chemically very similar silicone elastomers broke down electrically in very different ways. These observations emphasize that the modification of the silicone backbone may open up for completely new possibilities for stabilizing the silicone elastomer electrically. In order to tailor the elastomers, more knowledge is needed but these copolymers pave the first path towards a better understanding of the complex connection between electrical and thermal stability. Minor changes in the polymer backbone structure result in changes in electrical breakdown patterns and understanding why is crucial for enabling design for extraordinarily stable elastomers and thus ultimately reliable dielectric elastomer based products.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Electron Nanoscopy
Authors: Yu, L. (Intern), Mateiu, R. V. (Intern), Skov, A. L. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from International Conference on Electromechanically Active Polymer (EAP) transducers & artificial muscles, Cartagena, Spain.
Main Research Area: Technical/natural sciences
Silicone elastomers, Dielectric, Electrical breakdown, Voltage stabilization, Characterization
Electronic versions:
Liyun_Yu_EuroEAP2017_abstract.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Electrical Double-Layer and Ion Bridging Forces between Symmetric and Asymmetric Charged Surfaces in the Presence of Mono- and Divalent Ions

An atomic force microscope, employing the colloidal probe technique, was used to study the interactions between six different combinations of silane-functionalized silica surfaces in NaCl and CaCl₂ solutions. The surfaces consisted of monolayers of the apolar trimethoxo(octyl)silane, the positively charged (3-aminopropyl)trimethoxysilane, and the negatively charged (3-mercaptopropyl)trimethoxysilane. The interactions between the three symmetric systems, as well as between the three asymmetric combinations of surfaces, were measured and compared to calculated electrical double-
layer forces. The results demonstrated that the long-range interactions between the surfaces in all cases were dominated by double-layer forces, while short-range interactions, including adhesion, were dominated by ion bridging forces in the cases where both interaction surfaces favored adsorption of calcium ions. The study thus also demonstrates how surface force studies in mono- and divalent salt solutions can be used as an analytical tool for probing specific functional groups on heterogeneous surfaces.

General information
State: Published
Organisations: Department of Chemistry, Centre for oil and gas – DTU, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Liu, X. (Intern), Feilberg, K. L. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern), Thormann, E. (Intern)
Number of pages: 9
Pages: 4426-4434
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Langmuir
Volume: 33
Issue number: 18
ISSN (Print): 0743-7463
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.99 SJR 1.55 SNIP 1.188
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.686 SNIP 1.308 CiteScore 4.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.816 SNIP 1.391 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.895 SNIP 1.356 CiteScore 4.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.177 SNIP 1.382 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.051 SNIP 1.357 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.148 SNIP 1.4
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.156 SNIP 1.351
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.383 SNIP 1.34
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.449 SNIP 1.434
Electron microscope investigations of activated chalcopyrite particles via the FLSmidth® ROL process

Because of its unique semiconductor properties, the world’s most abundant copper mineral, chalcopyrite (CuFeS2), is refractory with respect to atmospheric leaching using traditional acidic ferric sulfate lixiviant. FLSmidth® has developed a novel approach manipulating lattice properties of semi-conducting minerals with the benefit of increasing chemical reactivity and dissolution kinetics. In the FLSmidth® Rapid Oxidative Leach (ROL) process, leach kinetics are still further enhanced by combining chemical and mechanical processes with the assistance of a Stirred Media Reactor. Due to the reduction in surface passivation problems associated with atmospheric leaching, this process is typically able to achieve copper recoveries exceeding 95% in 6 h. An important factor contributing to this extraordinary process performance is a mineral preconditioning step (the focus of this study), which uses between 0.1 and 5 mol percent of copper (II) to dope the lattice and thereby “activate” chalcopyrite. Since lattice restructuring can have such a dramatic influence on semiconductor reactivity, the associated physico-chemical phenomena are worth studying. In this regard, we investigate the relationship between chemical activation and deformation of the chalcopyrite crystal lattice through the use of electron microscopy. Although the activation process took only an hour and the extent of conversion was on the order of a few mol%, the lattice was found to be strained throughout the particle. This paper draws some insights into the impact of applying chemical activation as a pretreatment for mechanochemical processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), FLSmidth USA Inc.
Authors: Karcz, A. P. (Intern), Damø, A. J. (Intern), Illerup, J. B. (Intern), Rocks, S. (Ekstern), Dam-Johansen, K. (Intern), Chaiko, D. (Ekstern)
Number of pages: 10
Pages: 12044-12053
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Science
Volume: 52
Issue number: 20
ISSN (Print): 0022-2461
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Elemental analysis of various biomass solid fractions in biorefineries by X-ray fluorescence spectrometry

Elemental analysis by X-ray fluorescence spectrometry (XRF) of solid samples from a biorefinery process was performed to study the behaviour of mineral elements in a process involving hydrothermal pretreatment of biomass (wheat straw, corn stover, sugarcane bagasse, palm oil empty fruit bunches, poplar) followed by enzymatic hydrolysis and fermentation.
For all the different biomasses, the biorefinery process concentrated silicon, aluminium, and calcium in the solid fraction, while potassium and magnesium were solubilised in the process and removed from the solid fraction. Sodium concentrations were in general low and they only increased in case of addition during the process. No general tendencies were observed for phosphorus, sulphur, and iron concentrations. A prerequisite for XRF elemental analysis was defining an average chemical formula for the organic matrix of process biomass samples. Based on ultimate elemental analysis of all biomasses, the formula for biomass was \( \text{C}_6\text{H}_{8.4}\text{O}_{3.5} \), which was used for all types of samples (raw biomass, pretreated biomass, and lignin residue) and can be used in future XRF analysis of samples of similar process and biomass feedstock as those used in this study.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DONG Energy A/S
Authors: Le, D. M. (Intern), Sorensen, H. R. (Ekstern), Meyer, A. S. (Intern)
Pages: 70-76
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Biomass and Bioenergy
Volume: 97
ISSN (Print): 0961-9534
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.188 SNIP 1.368
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.521 SNIP 1.615 CiteScore 4.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.888 SNIP 1.985 CiteScore 4.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.678 SNIP 1.823 CiteScore 4.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.545 SNIP 1.743 CiteScore 3.66
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.793 SNIP 2.283 CiteScore 4.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.931 SNIP 2.254
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.743 SNIP 2.187
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.609 SNIP 2.073
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.454 SNIP 1.77
Energy efficiency as an example of cross-discipline collaboration in chemical engineering

This paper summarizes the round-table discussion that was held during the European Congress of Chemical Engineering (ECCE) in Nice, France, in October 2015 on this topic. The panellists come from different fields of chemical engineering and have thus brought in different perspectives. The objective was to determine paths for developing innovative approaches in view of process optimization. The terminology is a first obstacle that was clarified. Energy efficiency can be envisaged either by optimizing thermodynamic functions (entropy or exergy), more pragmatically by selecting the adequate unit operation or in a very general vision by considering all decision variables (i.e. including economic and political) that may have an impact on the final service provided to society. The second issue relates to improving collaboration among various actors. These may be defined in terms of type of responsibility (industrials, mostly market-driven, or academic), or in terms of discipline. The role of professional societies as the European Federation for Chemical Engineers (EFCE) is stressed as a promoter of collaboration between disciplines. Finally, once willingness for collaboration is identified, the final question is how it can lead to true innovation. The largest innovation potential is often found at the interface between fields. Yet, it often requires both an effort to explain the mutual challenges in a didactic manner, and the development of tools that make it possible to each partner to be efficient in his own field while being aware of the global goal and of the constraints of the others.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, IFP Energies nouvelles, Aix-Marseille University, Technische Universität Dortmund, Norwegian University of Science and Technology, Ecole Polytechnique Federale de Lausanne (EPFL), ProSim S.A.
Authors: de Hemptinne, J. (Ekstern), Ferrasse, J. (Ekstern), Górak, A. (Ekstern), Kjelstrup, S. (Ekstern), Marechal, F. (Ekstern), Baudouin, O. (Ekstern), Gani, R. (Intern)
Pages: 183–187
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Research and Design
Volume: 119
ISSN (Print): 0263-8762
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
Shale gas, like natural gas, contains H₂, CO₂, CH₄ and that light hydrocarbon gases need processing to separate the gases for conversion to higher value products. Currently, distillation based separation is employed, which is energy intensive. Hybrid gas separation processes, combining absorption and membranes together with distillation require less energy and have attracted much attention. With the property of non-volatility and good stability, ionic liquids (ILs) have been considered as new potential solvents for the absorption step. In order to solve
this problem, a systematic screening model for ILs is established by considering the needed properties for gas absorption process design. Rigorous thermodynamic model of IL-absorbed gas systems is established for process design-analysis. A strategy for hybrid gas separation process synthesis where distillation and IL-based absorption are employed for energy efficient gas processing is developed and its application is highlighted for a model shale gas processing case study.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CERE – Center for Energy Resources Engineering, Chinese Academy of Sciences  
Authors: Liu, X. (Intern), Liang, X. (Intern), Gani, R. (Intern), Zhang, X. (Ekstern), Zhang, S. (Ekstern)  
Pages: 421-426  
Publication date: 2017

**Host publication information**

Title of host publication: Proceedings of the 27th European Symposium on Computer Aided Process Engineering – ESCAPE 27  
Volume: 40  
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Editors: Espuña, A., Graells, M., Puigjaner, L.  
Series: Computer - Aided Chemical Engineering  
ISSN: 1570-7946  
Main Research Area: Technical/natural sciences  
Conference: 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 01/10/2017 - 01/10/2017  
Energy efficient, Gas separation, Ionic liquids, Process design, Screening  
DOI: 10.1016/B978-0-444-63965-3.50072-6  
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

**Environmental performance assessment of Napier grass for bioenergy production**

The industrial production of chemicals and energy carriers has grown enormously with the support of new technologies. A proper assessment is needed to provide broader aspects for long-term sustainability. The purpose of this study was to evaluate the environmental sustainability of a biorefinery based on lignocellulosic biomass feedstock using emergy analysis and to propose the method to minimize material consumption and waste. The concept of emergy is to express the record of all resources used by the biosphere in earlier steps to produce a product or service, in term of solar energy equivalence. This idea provides the quantitative indicators involving the resource use and the percent renewability of the systems. For the proposed biorefinery model, Napier grass (Pennisetum purpureum) grown in Thailand was used as lignocellulosic feedstock. An emergy assessment was performed in two parts, comprised of the evaluation of the feedstock cultivation and of a biorefinery producing liquid fuels, methanol, steam, electricity and other by products, i.e., high purity CO2, sulfur. The emergy results revealed that the bio-based products depend mostly on non-renewable resources used in both biomass cultivation and biorefinery stages. For Napier grass cultivation, most of the emergy support came from local resources in term of evapotranspiration of Napier grass (33%) and the diesel consumption during the cultivation process (21%). The emergy sustainability indicator of the cultivation was 0.81. The emergy sustainability indicator of the whole process from cultivation to biorefinery stages dropped to 0.25, since the biorefinery section required solely economic inputs of which most were non-renewable. In conclusion, the implementation of the integrated biorefinery concept could minimize material consumption and waste generation and it also has higher performance in terms of the emergy compared to other existing processes.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Chulalongkorn University  
Authors: Nimmanterdwong, P. (Ekstern), Chalermsinsuwan, B. (Ekstern), Østergård, H. (Intern), Piumsomboon, P. (Ekstern)  
Pages: 645-655  
Publication date: 2017  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Cleaner Production  
Volume: 165  
ISSN (Print): 0959-6526  
Ratings:  
BFI (2018): BFI-level 2
Enzymatic conversion of CO2 to CH3OH via reverse dehydrogenase cascade biocatalysis: Quantitative comparison of efficiencies of immobilized enzyme systems

A designed biocatalytic cascade system based on reverse enzymatic catalysis by formate dehydrogenase (EC 1.2.1.2), formaldehyde dehydrogenase (EC 1.2.1.46), and alcohol dehydrogenase (EC 1.1.1.1) can convert carbon dioxide (CO2)
to methanol (CH$_3$OH) via formation of formic acid (CH$_2$O$_2$H) and formaldehyde (CHOH) during equimolar cofactor oxidation of NADH to NAD$^+$. This reaction is appealing because it represents a double gain: (1) reduction of CO$_2$ and (2) an alternative to fossil fuel based production of CH$_3$OH. The present review evaluates the efficiency of different immobilized enzyme systems and reaction designs that have been explored for optimizing this sequential enzymatic conversion of CO$_2$ to CH$_3$OH, including multilayer microcapsules, bead scaffolds, cationic nanofibers, and membrane systems. The recent progress within efficient cofactor regeneration, protein engineering of the enzymes for robustness, and advanced uses of membrane systems for enzyme reuse and product separation are assessed for large scale implementation of this biocatalytic reaction cascade. Industrial realization of enzymatic CO$_2$ to CH$_3$OH conversion including the option for reaping of formaldehyde and formate during the reaction warrants innovative development. There is a particular need for development of i) better enzymes; ii) improved understanding of enzyme structure function aspects of reverse catalysis by dehydrogenases, iii) quantitative kinetic models of the enzymatic cascade reaction during simultaneous cofactor regeneration, iv) robust systems for regeneration of reducing equivalents.

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Authors: Marpani, F. B. (Intern), Pinelo, M. (Intern), Meyer, A. S. (Intern)
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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BFI (2008): BFI-level 1
Web of Science (2008): Indexed yes
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Enzymatic production of wheat and ryegrass derived xylooligosaccharides and evaluation of their in vitro effect on pig gut microbiota

This study examines enzymatic production of linear xylooligosaccharides (XOS) and branched arabinoxylooligosaccharides (AXOS) from monocotyledonous biomass, wheat straw and ryegrass, and compares the in vitro effects of these XOS and AXOS on pig gut microbiota. XOS and AXOS were obtained from the biomass by treatment with different endo-1,4-β-xylanases. XOS of DP2-6 from wheat straw, obtained after treatment with Aspergillus niger endo GH11, suppressed growth of Clostridium perfringens and resulted in a high level of lactic acid production when fermented in vitro by pig fecal microbiota. Analogously, XOS ryegrass produced in the same way also suppressed Cl. perfringens growth, and more so than the corresponding ryegrass AXOS, but AXOS exhibited a more pronounced stimulation of lactic acid bacteria growth than XOS. The prebiotic potential, i.e., suppression of Cl. perfringens and stimulation of lactic acid bacteria, for the ryegrass oligosaccharides was as follows: XOS, produced by A. niger endo-1,4-β-xylanase (GH 11) ≥ AXOS, produced by Thermotoga maritima and Cellvibrio mixtus endo-1,4-β-xylanase s (GH10) > AXOS, produced by Trichoderma viride and Aspergillus aculeatus endo-1,4-β-xylanase s (GH11). These results indicate that wheat straw as well as green grass biomass such as ryegrass have potential as new sources of putative prebiotics for pig feed.

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Enzyme discovery for tuber processing pulps

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Enzyme Enhanced Protein Recovery from Green Biomass Pulp
Globally, animal feed protein is a key factor for production of meat for human consumption. Protein for animal feed is in many parts of the world not available in sufficient amounts; demand is met only through import of feed protein. Such protein deficit can be minimized through optimized use of local protein resources based on upgrade from e.g. green plant biomass. In present work we consider different strategies for protein recovery from white clover and ryegrass screw press pulps, using aqueous extraction, as well as carbohydrases and proteases enhanced extraction. Protein recovery in these studies was determined as a yield of solubilized protein with regard to the total protein in a screw press pulp. Aqueous extraction at pH 8.0 resulted in approx. 40 % protein recovery, while proteases application (Savinase 16.0L, Novozymes) enabled twice higher protein yield. Application of plant cell wall degrading enzymes (Cellic CTec2 and Cellic HTec2, Novozymes) did not provide detectable protein recovery, while consecutive proteases treatment resulted in approx. 95 % protein yield. RuBisCO peptides were demonstrated by amino acid analysis to be the major component of white clover and ryegrass pulp proteolyzates, generated by Savinase 16.0L protease.

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Scopus rating (2013): SJR 0.731 SNIP 1.074 CiteScore 2.01
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Scopus rating (2011): SJR 0.512 SNIP 1.02 CiteScore 1.35
Enzyme recycling in lignocellulosic biorefineries

Commercial production of ethanol from lignocellulosic biomass is becoming a reality, but the next step is to diversify the process and produce chemicals and materials. These lignocellulosic biorefineries will in many cases rely on hydrolysis of biomass carbohydrates into monosaccharides – the sugar platform. Cellulases are the most important enzymes required in this process, but the complex nature of lignocellulose requires several other enzymes (hemicellulases and auxiliary enzymes) for efficient hydrolysis. Enzyme recycling increases the catalytic productivity of the enzymes by reusing them for several batches of hydrolysis, and thereby reduces the overall cost associated with the hydrolysis. Research on this subject has been ongoing for many years and several promising technologies and methods have been developed and demonstrated. But only in a very few cases have these technologies been upscaled and tested in industrial settings, mainly because of many difficulties with recycling of enzymes from the complex lignocellulose hydrolyzate at industrially relevant conditions, i.e., high solids loadings. The challenges are associated with the large number of different enzymes required for efficient hydrolysis, enzyme stability, and the detrimental interaction between enzyme and lignin. This review provides a comprehensive overview of the various methods for enzyme recovery and recycling, for example recycling of free enzymes, readsorption to fresh material, recycling of solids, membrane filtration, and immobilization. Lignin is a major obstacle for successful hydrolysis and enzyme recycling. A thorough understanding of this subject and possibilities to minimize adsorption or methods to desorb the enzymes are important in order to develop the technology.

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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.74 SNIP 1.704 CiteScore 3.92
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.821 SNIP 1.867 CiteScore 4.49
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Scopus rating (2012): SJR 1.487 SNIP 1.656 CiteScore 3.56
Establishment and calibration of consensus process model for nitrous oxide dynamics in water quality engineering

Research on biological nitrogen removal (BNR) in wastewater treatment plants (WWTP) has historically focused on achieving good effluent quality, with more recent attention to energy savings and carbon dioxide (CO2) footprints. Novel processes and operating conditions are being implemented that enhance cost and energy efficiency in BNR, while maintaining effluent quality. Now, increasing attention is placed on direct emissions of nitrous oxide (N2O) as by-product of BNR; N2O is a greenhouse gas (GHG) with a high warming potential and also an ozone depleting chemical compound.

Several N2O production pathways have been identified from pure culture studies, while mechanisms are still being unravelled. Heterotrophic bacteria (HB) and ammonium oxidizing bacteria (AOB) are well known to produce N2O. However, the effect of environmental factors on N2O production is not yet well understood. Current process modelling efforts aim to reproduce experimental data with mathematical equations, structuring our understanding of the system. Various mechanistic models with different structures describing N2O production have been proposed, but no consensus exists between researchers. Hence, the existing plant-wide GHG models still lack a complete biological process model that can be integrated in a methodology that assesses N2O emissions and their impact on overall plant performance. A mathematical model structure that describes N2O production during biological nitrogen removal is proposed. Two autotrophic and one heterotrophic biological pathways are coupled with abiotic processes. The model stoichiometry and process rates synthesize a comprehensive literature review on the metabolism of microbes involved in nitrogen removal. The proposed model can describe all relevant NO and N2O production pathways with fewer parameters than present in other proposed models. A novel experimental design based on the developed model and on extant respirometric techniques is introduced. Monitoring dissolved oxygen and N2O allowed the isolation of individual processes and the estimation of parameters associated to oxygen consumption (endogenous activity, nitrite and ammonium oxidation) and N2O production (NN, ND and HD pathway contributions). To estimate parameters of the N2O model a rigorous procedure is presented as a case study. The calibrated model predicts the NO and N2O dynamics at varying ammonium, nitrite and dissolved oxygen levels in two independent systems: (a) an AOB-enriched biomass and (b) activated sludge (AS) mixed liquor biomass. A total of ten (a) and seventeen (b) parameters are identified with high accuracy (coefficients of variation < 25%). The critical validation of the model response and the estimated parameter values represent a novel and rigorous tool for N2O modelling studies. For the first time, uncertainty associated with parameter estimation from N2O models is reported, this procedure is recommended to be included with best-fit simulations. Additionally, modelling electron competition in heterotrophic processes is explored via an analogy to current intensity through resistors in electric circuits. While further model validation is required, this approach captured the electron competition during denitrification for four different carbon sources. Overall, a combination of modelling and experimental efforts to study N2O dynamics was successfully implemented. Results represent a step forward in the development of consensus process model for N2O emissions in WQE processes.

General information

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Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Domingo-Felez, C. (Intern), Smets, B. F. (Intern), Plósz, B. G. (Intern), Sin, G. (Intern)
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Evaluation of equations of state for simultaneous representation of phase equilibrium and critical phenomena

Precise description of the critical points with association equations of state requires rescaling of the parameters to match experimental critical temperature and pressure of pure components. In this work we developed a method to include critical data restrictions in the parametrization procedure of the Cubic-Plus-Association (CPA) equation of state (EoS). We obtained new parameters for methanol and alkanes from n-hexane to n-decane. The comparison with the original parameters showed that this procedure is important for associating compounds, since for inert species the equation reduces to the Soave-Redlich-Kwong (SRK) EoS. The application of the rescaled parameters improved the critical point representation of pure fluids at the expense of the saturated liquid phase volume description. In the case of binary mixtures containing methanol and n-alkanes, the association model with the new parameters satisfactorily predicted the experimental critical data, indicating the importance of the rescaling parametrization procedure in the computation of the critical pressure and temperature for systems with associating species. Both sets of CPA parameters gave similar deviations in the bubble point pressure and vapor composition for the vapor-liquid equilibrium calculations. However, the rescaled parameters gave rise to larger deviations in the composition of the polar rich phase in the liquid-liquid equilibrium.
Evaluation of mixing and mass transfer in a stirred pilot scale bioreactor utilizing CFD

Knowledge and prediction of mixing and mass transfer in agitated bioreactors is fundamental for process development and scale up. In particular key process parameters such as mixing time and volumetric mass transfer coefficient are essential for bioprocess development. In this work the mixing and mass transfer performance of a high power agitated pilot scale bioreactor has been characterized using a novel combination of computational fluid dynamics (CFD) and experimental investigations. The effect of turbulence inside the vessel was predicted using a standard RANS k-ε model. Mixing time was investigated by carrying out sodium chloride tracer experiments for both Newtonian and non-Newtonian fluids at various viscosities and agitation speeds, while tracking the conductivity. The mixing performance was simulated with CFD and the results showed good agreement with the experimental data. The mass transfer coefficients were determined from six Trichoderma reesei fermentations at different well-defined process conditions. Similarly the mass transfer was predicted by Higbie's penetration model from two-phase CFD simulations using a correlation of bubble size and power input, and the overall mass transfer coefficients were in accordance with the experimental data. This work illustrates the possibility of predicting the two phase fluid dynamic performance of an agitated pilot scale bioreactor using validated CFD models. These models can be applied to illustrate the effect of changing the physical process conditions.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, LEO Pharma A/S, Novozymes A/S
Authors: Bach, C. (Intern), Yang, J. (Intern), Larsson, H. K. (Intern), Stocks, S. M. (Ekstern), Gernaey, K. (Intern), Albæk, M. O. (Ekstern), Krühne, U. (Intern)
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  Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
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  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
  Web of Science (2014): Indexed yes
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  Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
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  BFI (2012): BFI-level 2
  Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
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  BFI (2011): BFI-level 2
  Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
  ISI indexed (2011): ISI indexed yes
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  BFI (2010): BFI-level 2
  Scopus rating (2010): SJR 1.319 SNIP 1.708
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 2
  Scopus rating (2009): SJR 1.293 SNIP 1.759
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  Scopus rating (2008): SJR 1.299 SNIP 1.6
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  Scopus rating (2007): SJR 1.347 SNIP 1.523
  Web of Science (2007): Indexed yes
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  Web of Science (2006): Indexed yes
  Scopus rating (2005): SJR 1.445 SNIP 1.801
  Scopus rating (2004): SJR 1.301 SNIP 1.858
  Web of Science (2004): Indexed yes
  Scopus rating (2003): SJR 1.7 SNIP 1.676
  Web of Science (2003): Indexed yes
  Scopus rating (2002): SJR 1.675 SNIP 1.279
  Web of Science (2002): Indexed yes
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Evaluation of phosphorus in thermally converted sewage sludge: P pools and availability to wheat

Aims
Dried sewage sludge (SS) and the by-products of four SS thermal conversion processes (pyrolysis, incineration and two types of gasification) were investigated for phosphorus (P) availability.

Methods
A sequential extraction was used to determine the distribution of P among different P pools. After mixing materials with soil, availability of the P was determined with soil P extractions and in a growth experiment with wheat.

Results
Thermally converted SS contained a greater proportion of P within recalcitrant pools than dried SS. Despite having very different P pool distributions, the incinerated and dried SS provided similar amounts of P to plants. Plant P supply from dried and incinerated SS was lower than the comparable soluble P treatment (50 mg P kg⁻¹), but higher than a soluble treatment at a lower rate (20 mg P kg⁻¹). Plant P uptake in gasified and pyrolysed treatments was only marginally greater than uptake in a control (no P) treatment. Plant P uptake correlated most closely with diffusive gradients in thin films (DGT) P analysis of soil-material mixes. Phosphorus availability in the dried and incinerated SS treatments increased over time.

Conclusions
We propose that the dried and incinerated SS have potential as slow release P fertilisers in low pH soils.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Adelaide, University of Copenhagen
Authors: Mackay, J. E. (Ekstern), Cavagnaro, T. R. (Ekstern), Jakobsen, I. (Ekstern), Macdonald, L. M. (Ekstern), Grønlund, M. (Ekstern), Thomsen, T. P. (Intern), Müller-Stöver, D. S. (Ekstern)
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.357 SNIP 1.463 CiteScore 3.15
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.385 SNIP 1.653 CiteScore 3.5
Experimental and computational evaluation of area selectively immobilized horseradish peroxidase in a microfluidic device

A microreactor with a square shaped reactor chamber was developed with the aim to correlate enzyme positioning with biocatalytic activity. The enzyme position as an important parameter to improve the contribution of the individual enzymes towards the overall reactor efficacy was therefore evaluated experimentally and by computational fluid dynamics (CFD) simulations. Ultimately, such a correlation would lead to faster development through computational pre-screening and optimized experimental design.

In this proof-of-concept study, microreactors were prepared in a 2-step curing process of an off-stoichiometric thiol-ene-epoxy (OSTE+) mixture employing both a thiol-ene (TEC) and a thiol-epoxy curing reaction. Subsequent surface functionalization of the remaining thiol groups on the reactor surface through stenciled photoinitiated TEC enabled the preparation of specific surface patterns in the reactor. Patterns were visualized using an allyl-functional disperse red dye, illustrating the successful preparation of a fully reacted surface, a half covered surface and 2 checkerboard patterns. Similarly, allyl glycidyl ether was exploited to functionalize the microreactor surface with epoxide groups, which were used for covalent immobilization of horseradish peroxidase (HRP) in the same patterns. Biocatalytic activity measurements confirmed a clear dependency of the overall reactor performance depending on the spatial distribution of the immobilized enzymes, where specifically the two checkerboard motifs were identified as being particularly effective compared to enzymes covering homogeneously the entire reactor surface. The performance of the same configurations was additionally determined by 3-dimensional CFD simulations. The computational model predicted
the same tendencies for the overall reactor performance as obtained from experimental determination. This good agreement between the obtained experimental and computational results confirmed the high potential of CFD models for predicting and optimizing the biocatalytic performance of such a reactor.
Experimental and Modeling Investigation of the Effect of H2S Addition to Methane on the Ignition and Oxidation at High Pressures

The autoignition and oxidation behavior of CH4/H2S mixtures has been studied experimentally in a rapid compression machine (RCM) and a high-pressure flow reactor. The RCM measurements show that the addition of 1% H2S to methane reduces the autoignition delay time by a factor of 2 at pressures ranging from 30 to 80 bar and temperatures from 930 to 1050 K. The flow reactor experiments performed at 50 bar show that, for stoichiometric conditions, a large fraction of H2S is already consumed at 600 K, while temperatures above 750 K are needed to oxidize 10% methane. A detailed chemical kinetic model has been established, describing the oxidation of CH4 and H2S as well as the formation and consumption of organosulfuric species. Computations with the model show good agreement with the ignition measurements, provided that reactions of H2S and SH with peroxides (HO2 and CH3OO) are constrained. A comparison of the flow reactor data to modeling predictions shows satisfactory agreement under stoichiometric conditions, while at very reducing conditions, the model underestimates the consumption of both H2S and CH4. Similar to the RCM experiments, the presence of H2S is predicted to promote oxidation of methane. Analysis of the calculations indicates a significant interaction between the oxidation chemistry of H2S and CH4, but this chemistry is not well understood at present. More work is desirable on the reactions of H2S and SH with peroxides (HO2 and CH3OO) and the formation and consumption of organosulfuric compounds.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, DNV-GL Oil & Gas, Technical University of Denmark
Authors: Gersen, S. (Ekstern), van Essen, M. (Ekstern), Darmeveil, H. (Ekstern), Hashemi, H. (Intern), Rasmussen, C. T. (Ekstern), Christensen, J. M. (Intern), Glarborg, P. (Intern), Levinsky, H. (Ekstern)
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Scopus rating (2015): CiteScore 3.34
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BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
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BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
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Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
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Extensional Rheology and flow-induced crystallization of polyethylene above $T_m$

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Authors: Wingstrand, S. L. (Intern), Mortensen, K. (Ekstern), Huang, Q. (Intern), Shen, B. (Ekstern), Kornfield, J. A. (Ekstern), Imperialy, L. (Ekstern), Stepanyan, R. (Ekstern), Hassager, O. (Intern)
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Extension of modified RAND to multiphase flash specifications based on state functions other than (T,P)
The recently proposed modified RAND formulation is extended from isothermal multiphase flash to several other state function based flash specifications. The obtained general formulation is applicable to chemical equilibrium although this study is focused on flash with only phase equilibrium. It is demonstrated that a common symmetric Jacobian matrix can be formulated for all of these flash specifications. Newton iteration with the common Jacobian is used to converge for the majority of cases and a Q-function maximisation with nested isothermal flash in the inner loop is used for the non-convergent exceptions. For isothermal flash with modified RAND, it can happen in rare occasions that the modified RAND step is ascending in the Gibbs energy. A correction of the step is proposed for such cases to obtain a descent direction without violating the condition used in the derivation of modified RAND. A two-phase example is used to demonstrate that the described method is suitable for (H,P), (T,V), (S,V) and (U,V) flash specifications and a four-phase case is examined in more detail for the difficult (U,V) case. Two- and three-phase examples close to critical regions are used to demonstrate the effectiveness of the correction procedure for the modified RAND step and to show that satisfactory rates of convergence are obtained.
Facilitation of phosphorus uptake in maize plants by mycorrhizosphere bacteria

A major challenge for agriculture is to provide sufficient plant nutrients such as phosphorus (P) to meet the global food demand. The sufficiency of P is a concern because of its essential role in plant growth, the finite availability of P-rock for fertilizer production and the poor plant availability of soil P. This study investigated whether biofertilizers and bioenhancers, such as arbuscular mycorrhizal fungi (AMF) and their associated bacteria could enhance growth and P uptake in maize. Plants were grown with or without mycorrhizas in compartmented pots with radioactive P tracers and were inoculated with each of 10 selected bacteria isolated from AMF spores. Root colonization by AMF produced large plant growth responses, while seven bacterial strains further facilitated root growth and P uptake by promoting the development of AMF extraradical mycelium. Among the tested strains, Streptomyces sp. W94 produced the largest increases in uptake and translocation of 33P, while Streptomyces sp. W77 highly enhanced hyphal length specific uptake of 33P. The positive relationship between AMF-mediated P absorption and shoot P content was significantly influenced by the bacteria inoculants and such results emphasize the potential importance of managing both AMF and their microbiota for improving P acquisition by crops.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, University of Pisa
Authors: Battini, F. (Ekstern), Grønlund, M. (Intern), Agnolucci, M. (Ekstern), Giovannetti, M. (Ekstern), Jakobsen, I. (Intern)
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Main Research Area: Technical/natural sciences
Publication information
Journal: Scientific Reports
Volume: 7
Issue number: 1
Article number: 4686
ISSN (Print): 2045-2322
Ratings:
BFI (2018): BFI-level 1
Fermentative production of butyric acid from wheat straw: Economic evaluation

The economic feasibility of biochemical conversion of wheat straw to butyric acid was studied in this work. Basic process steps included physicochemical pretreatment, enzymatic hydrolysis and saccharification, fermentation with in-situ acids separation by electrodialysis and product purification. Two scenarios (S1 and S2) were examined assuming a plant with an annual capacity of 10,000 tonnes of product installed in India (due to significantly lower feedstock prices). S1 resulted in a product of 89% butyric acid mixed with acetic acid and S2 produced butyric acid of 99% purity. Unit production cost was estimated at 2.75 and 3.31 $ per kg product for S1 and S2 respectively. The main part of production cost was attributed to steam for the purification step and electricity for the in-situ acids separation. This unit production cost combined with an estimated butyric acid selling price (year 2014) at 3.50 and 3.95 $ per kg product (for S1 and S2 respectively) and a plant capacity of 10,000 tonnes indicated an internal rate of return of 14.92% and 12.42% and payback time of 4.28 and 4.70 years for S1 and S2 respectively. Sensitivity analysis showed that under the assumptions of the present study the optimum plant capacity would lie between 10,000 and 15,000 tonnes of product per year.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, PILOT PLANT, Aalborg University
Authors: Baroi, G. N. (Ekstern), Gavala, H. N. (Intern), Westermann, P. (Ekstern), Skiadas, I. (Intern)
Pages: 68-80
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Volume: 104
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
Field study of the long-term release of block copolymers from fouling-release coatings

The addition of block copolymers (i.e., oils) is a common technique to enhance the biofouling-resistance properties of poly(dimethylsiloxane) (PDMS)-based fouling-release coatings. These copolymers diffuse from the bulk to the surface of...
the coating, thus modifying the properties of the surface and providing fouling-resistance properties. Upon release, dissolvoion or degradation of copolymer molecules at the surface, new molecules can diffuse from the bulk of the coating and cover the surface. Therefore, the long-term performance of these coatings is dependent on the stability and release rate of copolymer molecules from the surface. A method was developed to quantify the concentration of PDMS-based block copolymers from fouling-release coatings. About 300 experimental coatings exposed to seawater for up to 5.2 years were included in the analysis. The results showed that the loss of copolymer (in % on a weight basis) is significantly higher in warm waters, while the initial copolymer concentration in the coating does not have any effect for copolymer concentrations between 1 and 7 wt%. In short-term exposure, it was found that loss of copolymer was much higher in coatings containing small amounts of an organic biocide (copper pyrithione). Conversely, biocide-containing coatings displayed larger copolymer retention values in long-term experiments. Opposite results were obtained for biocide-free coatings, suggesting that the addition of the organic biocide alters the release profile of copolymers from fouling-release coatings. Finally, the potential of long-term field-studies is discussed, as compared to short-term laboratory experiments usually performed within fouling-release coatings studies.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Danish Polymer Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Hempel A/S
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.89 SJR 0.852 SNIP 1.3
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.849 SNIP 1.39 CiteScore 2.84
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.992 SNIP 1.566 CiteScore 2.8
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.03 SNIP 1.663 CiteScore 2.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.043 SNIP 1.862 CiteScore 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.884 SNIP 1.606 CiteScore 2.34
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.983 SNIP 1.537
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.867 SNIP 1.333
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
First Study of Poly(3-Methylene-2-Pyrrolidone) as a Kinetic Hydrate Inhibitor

Formation of gas hydrates is a problem in the petroleum industry where the gas hydrates can cause blockage of the flowlines. Kinetic hydrate inhibitors (KHIs) are water-soluble polymers, sometimes used in combination synergistically or with non-polymeric synergists, that are used to prevent gas hydrate blockages. They have been used in the field successfully since 1995. In this paper, we present the first KHI results for the polymer, poly(3-methylene-2-pyrrolidone) (P(3M2P)), which is structurally similar to poly(N-vinylpyrrolidone) (PVP), one of the first KHIs to be discovered. 3M2P polymers with different molecular weights (5500 and 2500 g/mole) and at different concentrations (2500, 5000 and 7500 ppm) were investigated for their KHI performance on SII hydrates in high-pressure rocking cells. We also investigated the synergistic effect of P(3M2P) with n-butyl glycol ether (BGE), a known synergist for some KHI polymers. At the lower concentrations, P(3M2P) gives a similar performance to PVP (Mw = 8000-9000 g/mole). However, PVP outperforms both samples of P(3M2P) at 7500 ppm, with and without BGE. We suggest that the reasons for the performance level of P(3M2P) are related to greater resonance stabilization of the amide group in P(3M2P) compared to PVP. Also, the pyrrolidone ring of the PVP repeat unit has a larger hydrophobic sequence of three methylene units compared to the two methylene units in the pyrrolidone ring of P(3M2P). This relates well to previous studies where larger hydrophobic groups are preferable in KHI polymers as long as they are water-soluble at hydrate-forming temperatures.

General information
State: Published
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2

Block copolymers, Fouling-release coatings, Oils, Release

DOI: 10.1016/j.porgcoat.2017.07.001
Source: FindIt
Source-ID: 2372680570
Publication: Research - peer-review › Journal article – Annual report year: 2017
Flooding of North Sea chalk and greensand cores with specific brines

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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
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DOI: 10.1021/acs.energyfuels.7b03006
Publication: Research - peer-review › Poster – Annual report year: 2017
Flow characterization of aerated bubble column reactor using electrical resistance tomography and computational fluid dynamic methods

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Center for Process Engineering and Technology, Ryerson University
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Number of pages: 1
Publication date: 2017
Event: Abstract from 10th World Congress of Chemical Engineering (WCCE10), Barcelona, Spain.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2018

Fly Ash Formation during Suspension-Firing of Biomass. Effects of Residence Time and Fuel-Type

The objective of this work was to generate comprehensive data on the formation of residual fly ash during the initial stages of suspension-firing of biomass. Combustion experiments were carried out with pulverized biomass fuels (two straw fuels and two wood fuels), in an entrained flow reactor at 1200-1400 °C, simulating full-scale suspension-firing of biomass. By the use of a movable, cooled and quenched gas/particle sampling probe, samples were collected at different positions along the vertical axis in the reactor, corresponding to gas residence times ranging from 0.25 – 2.0s. The collected particles were subjected to various analyses, including char burnout level, particle size distribution, elemental composition, and particle morphology and composition. Furthermore, the transient release, i.e. the vaporization of the flame-volatile inorganic elements K, Cl and S, from the burning fuel particles to the gas phase, has been quantified by using two different calculation methods. The ash formation mechanisms were found to be quite similar for straw and wood. The degree of conversion (char burn-out level) was generally good at residence times ≥ 1s. The size distribution of the residual fly ash particles evolved with residence time. For all ashes at long residence times a peak of residual ash particles in the range of 20 – 100 µm was observed. The residual ash particles were rich in Si, K and Ca. Further, at long residence times, submicron particles consisting primarily of KCl (condensed aerosols) became abundant in the ashes from straw combustion. Release of K to the gas phase was nearly 100 % for the two wood fuels and one of the straw fuels. A straw sample (Straw 2) with high Si/K molar ratio and a relative shortage of Ca showed a limited release of K in the range of 65 %; this suggests larger retention of K in Si-rich, Ca-lean fuels, due to incorporation of K into silicate structures. All S and Cl were nearly completely released to the gas phase for all studied samples.

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Damø, A. J. (Intern), Jensen, P. A. (Intern), Jappe Frandsen, F. (Intern), Wu, H. (Intern), Glarborg, P. (Intern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
Fracture in Soft Materials

Fracture is a phenomenon that is generally associated with solids. A key element in fracture theory is the so-called weakest link idea that fracture initiates from the largest pre-existing material imperfection. However, recent work has demonstrated that fracture can also happen in liquids, where surface tension will act to suppress such imperfections. Therefore, the weakest link idea does not seem immediately applicable to fracture in liquids. This presentation will review fracture in liquids and argue that fracture in soft liquids is a material property independent of pre-existing imperfections. The following questions then emerge: What is the material description needed to predict crack initiation, crack speed and crack shape in soft materials and liquids.

Freezing Point Determination of Water–Ionic Liquid Mixtures

Freezing points of aqueous solutions of HOEtpyBr, HOEtmmBr, AmimCl, EtOMmmCl, EmimDep, and EmimAc were measured using a modified Beckmann apparatus with automatic data logging. The ionic liquids (ILs) in this study exhibited
features similar to those of inorganic salts in depressing the freezing point of water. On the basis of the cryoscopic behavior recorded, the solid phases formed at higher IL contents were presumed to be hydrates of the form IL·nH₂O. The HEOtPrBr+H₂O and HEOtMimBr+H₂O systems formed simple eutectic systems. The eutectic points were found to be at a water mole fraction of 0.617 and 219.841 K in the first system and at a water mole fraction of 0.657 and 202.565 K in the second system. Water activities in aqueous IL solutions were predicted by COSMO-RS and COSMO-SAC and compared to water activities derived from the experimentally determined freezing points. The COSMO-RS predictions were closer to the experimental water activities than the COSMO-SAC predictions. The experimental results indicate that the freezing points of IL+H₂O systems are affected by the nature of both cations and anions. However, according to the COSMO-RS excess enthalpy predictions, the anions have a relatively higher influence than cations on the IL+H₂O interaction.

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, CERE – Center for Energy Resources Engineering, Chinese Academy of Sciences
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Pages: 2374–2383
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.054 SNIP 1.299
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.313 SNIP 1.037
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Full-scale Milling Tests of Wood Pellets for Combustion in a Suspension-Fired Power Plant Boiler

The size reduction of pelletized wood is crucial in suspension-fired power plants, and hence its milling characteristics are of interest to optimize the milling and combustion process. The objective of the study was to compare the size and shape of pellets disintegrated in hot water with that from pellets comminuted at different mill loads. The milling performance of two industrial wood pellet qualities in large-scale coal vertical roller mills at different mill operating conditions was studied. The milling performance was assessed by determining the specific grinding energy consumption (SGEC), and analyzing the comminuted particle shape and particle size distribution (PSD). Large-scale pellet comminution produced finer and wider PSDs than pellet disintegration in hot water, but only slightly altered the particle shape. The mill pressure loss, absorbed mill power, and hence SGEC depended on the pellet quality. Decreasing the mill load produced finer and wider PSDs, and reduced the mill pressure loss and absorbed mill power. However, the SGEC was negatively correlated with the mill load. Adjustments of mill operating conditions had a minor effect on the comminuted particle shape.

Functional hydrocolloids from seaweeds

The global production of seaweeds continues to grow for production of food hydrocolloids, i.e. carbohydrate polymers that form viscous suspensions and gels in water. Because of their unique gelling properties seaweed hydrocolloids are used in various food and pharmaceutical applications. Asian countries and Tanzania are currently the main producers of seaweed hydrocolloids based on cultivation of seaweeds such as Kappaphycus alvarezi, Gracilaria spp. and Laminaria spp. that hold carrageenan, agar, and alginate, respectively. In this review we summarize the chemistry, food uses, and gelling mechanisms of carrageenan, agar, and alginate, and describe the key techniques and principles for their extraction from seaweeds. We also discuss the options for local seaweed manufacturing as a business opportunity in countries along the West African coast.
Fungal Enzymes and Yeasts for Conversion of Plant Biomass to Bioenergy and High-Value Products

Fungi and fungal enzymes play important roles in the new bioeconomy. Enzymes from filamentous fungi can unlock the potential of recalcitrant lignocellulose structures of plant cell walls as a new resource, and fungi such as yeast can produce bioethanol from the sugars released after enzyme treatment. Such processes reflect inherent characteristics of the fungal way of life, namely, that fungi as heterotrophic organisms must break down complex carbon structures of organic materials to satisfy their need for carbon and nitrogen for growth and reproduction. This chapter describes major steps in the conversion of plant biomass to value-added products. These products provide a basis for substituting fossil-derived fuels, chemicals, and materials, as well as unlocking the biomass potential of the agricultural harvest to yield more food and feed. This article focuses on the mycological basis for the fungal contribution to biorefinery processes, which are instrumental for improved resource efficiency and central to the new bioeconomy. Which types of processes, inherent to fungal physiology and activities in nature, are exploited in the new industrial processes? Which families of the fungal kingdom and which types of fungal habitats and ecological specializations are hot spots for fungal biomass conversion? How can the best fungal enzymes be found and optimized for industrial use? How can they be produced most efficiently-in fungal expression hosts? How have industrial biotechnology and biomass conversion research contributed to mycology and environmental research? Future perspectives and approaches are listed, highlighting the importance of fungi in development of the bioeconomy.

General approach for solving the density gradient theory in the interfacial tension calculations
Within the framework of the density gradient theory, the interfacial tension can be calculated by finding the density profiles that minimize an integral of two terms over the system of infinite width. It is found that the two integrands exhibit a constant difference along the interface for a finite planar interface, and this difference becomes smaller as the interface width increases. These findings naturally lead to a solution procedure that consists of an inner loop and an outer loop for calculating the interfacial tension of a planar interface. The outer loop deals with the relationship between the interfacial tension and the interface width, and it permits us to obtain accurate results from finite width calculations. The inner loop minimizes the interfacial tension for a given interface width by adjusting the density profiles, in which the integrals are evaluated by a combination of Gauss-Lobatto quadrature and Lagrange interpolation based polynomial approximation. A better approximation of the interfacial tension is derived by a path integration along the density profiles. These strategies enable us to obtain accurate solutions with looser tolerance criteria and a fewer number of thermodynamic property evaluations compared to other methods. The performance of the algorithm with recommended parameters is analyzed for various systems, and the efficiency is further compared with the geometric-mean density gradient theory, which only needs to solve nonlinear algebraic equations. The results show that the algorithm is only 5-10 times less efficient than
solving the geometric-mean density gradient theory.

**General Information**
- State: Published
- Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, KT Consortium
- Authors: Liang, X. (Intern), Michelsen, M. L. (Intern)
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- Volume: 451
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  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 2
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 2
  - Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
    - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 2
  - Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
    - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 2
  - Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
    - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 2
  - Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
    - ISI indexed (2013): ISI indexed yes
    - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 2
  - Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
    - ISI indexed (2012): ISI indexed yes
    - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 2
  - Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
    - ISI indexed (2011): ISI indexed yes
    - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 0.986 SNIP 1.317
    - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 2
  - Scopus rating (2009): SJR 1.133 SNIP 1.164
    - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 1
  - Scopus rating (2008): SJR 1.227 SNIP 1.09
    - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 1.031 SNIP 1.151
    - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 1.034 SNIP 1.245
    - Web of Science (2006): Indexed yes
  - Scopus rating (2005): SJR 1.009 SNIP 1.3
    - Web of Science (2005): Indexed yes
General approach to characterizing reservoir fluids for EoS models using a large PVT database

Fluid characterization is needed when applying any EoS model to reservoir fluids. It is important especially for non-cubic models such as PC-SAFT where fluid characterization is less mature. Furthermore, there is a great interest to apply non-cubic models to high pressure high temperature reservoir fluids as they are believed to give better description of density and compressibility over a wide temperature and pressure range. We proposed a general approach to characterizing reservoir fluids and applied it to PC-SAFT. The approach consists in first, developing the correlations based on the DIPPR database, and then adjusting the correlations based on a large PVT database. The adjustment was made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and stock tank oil densities, while keeping the n-alkane limit of the correlations unchanged. The general approach can also be applied to other EoS models for improving their fluid characterization and we showed this for SRK and PR. In addition, we developed a PNA based characterization method for PC-SAFT based on the same general principles. We made a comprehensive comparison in PVT calculation involving 17 EoS-characterization combinations and 260 reservoir fluids. The new characterization methods generally improved the PVT calculation results.
Motivated by industrial demands and ongoing scientific discoveries, continuous efforts are made to identify and create improved biocatalysts dedicated to plant biomass conversion. α-1,2 and α-1,3 arabinofuranosyl specific α-l-arabinofuranosidases (EC 3.2.1.55) are debranching enzymes catalyzing hydrolytic release of α-l-arabinofuranosyl residues, which decorate xylan or arabinan backbones in lignocellulosic and pectin constituents of plant cell walls. The CAZy database classifies α-l-arabinofuranosidases in Glycoside Hydrolase (GH) families GH2, GH3, GH43, GH51, GH54 and GH62. Only GH62 contains exclusively α-l-arabinofuranosidases and these are of fungal and bacterial origin. Twenty-two GH62 enzymes out of 223 entries in the CAZy database have been characterized and very recently new knowledge was acquired with regard to crystal structures, substrate specificities, and phylogenetics, which overall provides novel insights into structure/function relationships of GH62. Overall GH62 α-l-arabinofuranosidases are believed to play important roles in nature by acting in synergy with several cell wall degrading enzymes and members of GH62 represent...
promising candidates for biotechnological improvements of biofuel production and in various biorefinery applications.

**General information**

State: Published
Organisations: Department of Biotechnology and Biomedicine, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Enzyme and Protein Chemistry, CNRS, Aix Marseille Universite
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- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 11.05 SJR 2.681 SNIP 3.146
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 2.919 SNIP 3.432 CiteScore 10.56
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 2.922 SNIP 3.757 CiteScore 10.24
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 2.936 SNIP 4.028 CiteScore 10.71
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 3.552 SNIP 5.178 CiteScore 11.65
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 3.126 SNIP 4.726 CiteScore 10.75
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 2.928 SNIP 3.953
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 2.248 SNIP 3.162
- Scopus rating (2006): SJR 1.727 SNIP 3.036
- Scopus rating (2005): SJR 1.607 SNIP 2.949
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.063 SNIP 2.238
- Scopus rating (2003): SJR 1.215 SNIP 2.109
- Scopus rating (2002): SJR 0.851 SNIP 1.873
- Scopus rating (2001): SJR 0.573 SNIP 1.006
- Scopus rating (2000): SJR 0.121 SNIP 1.044
Guidelines for automated control systems for stoves

ERA-NET Bioenergy is a network of national research and development programmes focusing on bioenergy which includes 14 funding organisations from 10 European countries: Austria, Denmark, Finland, France, Germany, Ireland, The Netherlands, Poland, Sweden and the United Kingdom. Its mission is to enhance the quality and cost-effectiveness of European bioenergy research programmes, through coordination and cooperation between EU Member States. The project Woodstoves2020 (Development of next generation and clean wood stoves) has been supported in the period between October 2009 and September 2012 by ERA-NET Bioenergy under 7th Joint Call for Research and Development of the ERA-NET Bioenergy from 2013.

Today small-scale biomass combustion is one of the most relevant bioenergy applications. Driven by EU-wide and national measures to promote the utilisation of biomass for energy production, the European market for biomass based residential heating systems is expected to substantially increase by about 130% until 2020 (based on 2009). Regarding the installed units stoves show the highest and steadily increasing numbers in Europe. According to market studies performed within the EU FP7 project EU-UltraLowDust (Project No. 268189), in 2020 in Europe a potential for an annual installation of almost 2,200,000 stoves (logwood and pellet stoves) is forecasted.

This additional potential for renewable energy production will of course contribute to a reduction of the EU greenhouse gas emissions. However, it is also well known that among the different residential biomass combustion technologies logwood stoves show the highest CO, OGC and fine particulate matter (PM) emissions.

Against this background, the project Woodstoves2020 aims at the development of innovative measures and technologies in order to further reduce emissions from wood stoves, to increase their thermal efficiency and to expand their field of application from solely single room heating to central heating. The latter could especially be of relevance for future applications in low energy buildings.

Accordingly, the detailed objectives of the project proposed can be structured as follows.

Objectives related to emission reduction

-Development and implementation of automated control systems for stoves as a feature of new stoves but also as retrofit units for existing models. Automated control systems can help to widely eliminate user induced operation errors and therefore have a huge potential for emission reduction.

-Evaluation and test of new high-temperature catalysts specially adapted to wood stoves for efficient CO, OGC and soot emission reduction. Catalysts should be implemented in new stove concepts as a basis for an ultra-low emission operation which could be comparable to the emission level of automated small-scale boilers.

-Evaluation and test of foam ceramic materials for efficient PM emission reduction.

-Evaluation of the implementation of modern chimney draught regulators.

Objectives related to increasing efficiency and new fields of application

-Development and evaluation of efficient and novel heat storage options for stoves such as the application of PCM (phase change material) with high heat storage potential.

-Investigations regarding efficient heat recovery from stoves (increase of efficiency by the implementation of heat storage
units or measures to stabilise the draft or to reduce standing losses).

Objectives related to the implementation and evaluation of the different measures
- Test of the most promising concepts by performing test runs with prototypes.
- Development of design guidelines for stove manufacturers based on the evaluation of the new technologies tested towards a clean stove technology 2020.
- Development of guidelines for the implementation and retrofit of selected measures for old stoves.

With the new technologies developed within the project an emission reduction between 50 and 80% and an increase of the efficiencies in a range above 90% shall be possible. If in future all newly installed wood stoves in Europe would be equipped with these new technologies, a PM emission reduction of 60 - 90% could be achieved.

In order to reach these objectives, a consortium of 4 research organisations and 4 industrial partners from 4 European countries collaborated within Woodstoves2020 (see next page). This document summarises the outcomes of the investigations regarding the improvement of wood stoves by the application of automated control concepts as a primary measure for emission reduction. It should support stove manufacturers concerning the optimisation of their products and the development and design of new products with its recommendations which have been worked out based on scientific investigations as well as comprehensive test runs.

**General information**

**State:** Published

**Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, BIOS Bioenergisysteme GmbH, TFZ - Technology and Support Centre, Research Institutes of Sweden, NIBE Sweden AB, Kutzner + Weber GmbH

**Authors:** Illerup, J. B. (Intern), Mandl, C. (Ekstern), Obernberger, I. (Ekstern), Mack, R. (Ekstern), Hartmann, H. (Ekstern), Schüßler, I. (Ekstern), Furborg, J. (Ekstern), Illerup, J. B. (Intern), Volz, F. (Ekstern)

**Number of pages:** 28

**Publication date:** 2017

**Publication information**

**Place of publication:** Graz

**Publisher:** BIOS BIOENERGIESYSTEME GmbH

**Original language:** English

**Main Research Area:** Technical/natural sciences

**Electronic versions:**

Guidelines_Control_final.pdf

**Bibliographical note**


**Source:** PublicationPreSubmission

**Source-ID:** 140727991

Publication: Research › Report – Annual report year: 2017

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**Heat transfer corrected isothermal model for devolatilization of thermally-thick biomass particles**

Isenthalp model used in current computational fluid dynamic (CFD) model neglect the internal heat transfer during biomass devolatilization. This assumption is not reasonable for thermally-thick particles. To solve this issue, a heat transfer corrected isothermal model is introduced. In this model, two heat transfer corrected coefficients: HT-correction of heat transfer and HR-correction of reaction, are defined to cover the effects of internal heat transfer. A series of single biomass devolatilization case have been modeled to validate this model, the results show that devolatilization behaviors of both thermally-thick and thermally-thin particles are predicted reasonable by using heat transfer corrected model, while, isothermal model overestimate devolatilization rate and heating rate for thermally-thick particle. This model probably has better performance than isothermal model when it is coupled with CFD to model devolatilization of thermally-thick biomass particles.

**General information**

**State:** Published

**Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST)

**Authors:** Luo, H. (Intern), Wu, H. (Intern), Lin, W. (Intern), Dam-Johansen, K. (Intern)

**Number of pages:** 12

**Publication date:** 2017


**Main Research Area:** Technical/natural sciences

**Electronic versions:**

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Publication: Research - peer-review › Paper – Annual report year: 2017
Helbredstjek af dansk sundhedsteknologi: Sektorudviklingsrapport

Sådan kan samarbejde mellem industrien, universiteterne og sundhedsvæsenet skabe gode løsninger til forebyggelse, diagnostik, patientbehandling og rehabilitering

General information
State: Published
Organisations: Office for Innovation & Sector Services, Copenhagen Center for Health Technology, Department of Applied Mathematics and Computer Science, Embedded Systems Engineering, Center for Energy Resources Engineering, Scientific Computing, Department of Management Engineering, Technology and Innovation Management, Department of Electrical Engineering, Biomedical Engineering, Department of Micro- and Nanotechnology, Nano Bio Integrated Systems, Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Energy Conversion and Storage, Electrofunctional materials, IT Service, National Space Institute, Innovation and Research-based consultancy, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Office for Research and Relations, It-branchen, manjourn.dk
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Main Research Area: Technical/natural sciences
Electronic versions: 2017.02.16.DTU_Sektorudviklingsrapport_Helbredstjek_af_dansk_sundhedsteknologi.pdf
Publication: Commissioned › Report – Annual report year: 2017

High efficient conversion of furfural to 2-methylfuran over Ni-Cu/Al2O3 catalyst with formic acid as a hydrogen donor
Conversion of furfural to 2-methylfuran over Cu/Al2O3, Ni/Al2O3 and Ni-Cu/Al2O3 catalysts were investigated with formic acid as a hydrogen donor. Ni/Al2O3 showed a high catalytic activity but a moderate selectivity to 2-methylfuran. Contrarily, Cu/Al2O3 showed a low catalytic activity but a high selectivity for carbonyl reduction. Over the bimetallic catalysts Ni-10%Cu/Al2O3, by increasing Ni content, more furfural was converted with the reduction of carbonyl primarily. The effect of reaction solvent and the fraction of formic acid were also studied. The result showed that isopropanol solvent could contribute to the formation of furfuryl alcohol with 96% selectivity through the transfer hydrogenation process. Formic acid could decompose to H2 and CO2, remarkably promoting the hydrogenolysis of furfuryl alcohol to 2-methylfuran. Finally, 100% conversion and 92 mol% yield of 2-methylfuran could be obtained over 10%Ni-10%Cu/Al2O3. It was attributed to the synergic effect of Ni-Cu metals, with increased affinity for carbonyl reduction.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Chinese Academy of Sciences
Authors: Fu, Z. (Ekstern), Wang, Z. (Ekstern), Lin, W. (Intern), Song, W. (Ekstern), Li, S. (Ekstern)
Pages: 248-255
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
Journal: Applied Catalysis A: General
Volume: 547
ISSN (Print): 0926-860X
Ratings: BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.178 SNIP 1.311
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.203 SNIP 1.394 CiteScore 4.08
High-performance removal of acids and furans from wheat straw pretreatment liquid by diananofiltration

Two model solutions and a real stream from the hydrothermal pretreatment of wheat straw were subjected to nanofiltration, and permeate flux, retention and resistance to fouling were evaluated. Three commercial NF membranes were tested, and a pressure of 4 bars (range: 1–20 bars) and a temperature of 20°C (range: 20–50°C) were found to provide the best results in terms of retention. A subsequent nanodiafiltration consisting of five cycles enabled one to recover 90% of the monosaccharides (purity >99%). This result showed that diananofiltration could be a promising strategy for the recovery of high-purity streams of monosaccharides from pretreatment liquids.
High-pressure oxidation of ethane

Ethane oxidation at intermediate temperatures and high pressures has been investigated in both a laminar flow reactor and a rapid compression machine (RCM). The flow-reactor measurements at 600–900 K and 20–100 bar showed an onset temperature for oxidation of ethane between 700 and 825 K, depending on pressure, stoichiometry, and residence time. Measured ignition delay times in the RCM at pressures of 10–80 bar and temperatures of 900–1025 K decreased with increasing pressure and/or temperature. A detailed chemical kinetic model was developed with particular attention to the peroxide chemistry. Rate constants for reactions on the C₂H₅O₂ potential energy surface were adopted from the recent theoretical work of Klippenstein. In the present work, the internal H-abstraction in CH₃CH₂OO to form CH₂CH₂OOH was treated in detail. Modeling predictions were in good agreement with data from the present work as well as results at elevated pressure from literature. The experimental results and the modeling predictions do not support occurrence of NTC behavior in ethane oxidation. Even at the high-pressure conditions of the present work where the C₂H₅ + O₂ reaction yields ethylperoxyl rather than C₂H₂ + HO₂, the chain branching sequence CH₃CH₂OOCH₂CH₂OOH + O₂OOCH₂CH₂OOH → branching is not competitive, because the internal H-atom transfer in CH₃CH₂OO to CH₂CH₂OOH is too slow compared to thermal dissociation to C₂H₄ and HO₂.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Technical University of Denmark, DNV-GL Oil & Gas, Argonne National Laboratory
Pages: 150–166
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Main Research Area: Technical/natural sciences

Publication information
Journal: Combustion and Flame
Volume: 182
ISSN (Print): 0010-2180
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.41 SJR 1.125 SNIP 2.165
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.919 SNIP 2.448 CiteScore 5.12
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.388 SNIP 2.347 CiteScore 3.78
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.925 SNIP 2.639 CiteScore 4.85
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.43 SNIP 2.88 CiteScore 4.12
High pressure phase equilibrium of ternary and multicomponent alkane mixtures in the temperature range from (283–473) K

Asymmetric multicomponent alkane mixtures can be used as model systems for reservoir fluids. We have prepared two ternary mixtures, methane/n-butane/n-decane and methane/n-butane/n-dodecane, and two multicomponent mixtures composed of methane/n-butane/n-octane/n-dodecane/n-hexadecane/n-eicosane as model reservoir fluids and measured their phase equilibrium in the temperature range from (283–473) K by using a variable volume cell with full visibility. Their phase envelopes and liquid volume fractions below the saturation pressure have been measured. Four equations of state, including Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT), and Soave-Benedict-Webb-Rubin (Soave-BWR), have been used to predict phase equilibrium of the measured systems. PR and PC-SAFT give better results than others and Soave-BWR gives poor phase envelope predictions which are quite distinct from the predictions by other models. It is generally challenging for any of the tested models to predict all the measured phase envelopes with high accuracy. For predictive calculation of the liquid fractions, the agreement in the low pressure region is good whereas the fractions just below the saturation pressures are difficult to predict. Moreover GERG-2008 has also been tested with the measured methane/n-butane/n-decane system. It over predicts the saturation pressures but predicts low pressure liquid fractions quite accurately.
Publication information
Journal: Fluid Phase Equilibria
Volume: 449
ISSN (Print): 0378-3812
Ratings:
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  - Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
  - Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
  - Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
  - Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
  - Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
  - Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
  - Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
  - Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
  - Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
  - Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
  - Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 0.986 SNIP 1.317
  - Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
  - Scopus rating (2009): SJR 1.133 SNIP 1.164
  - Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
  - Scopus rating (2008): SJR 1.227 SNIP 1.09
  - Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.031 SNIP 1.151
  - Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.034 SNIP 1.245
  - Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.009 SNIP 1.3
  - Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 0.985 SNIP 1.349
  - Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 1.193 SNIP 1.301
  - Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 0.722 SNIP 1.101
  - Web of Science (2002): Indexed yes
- Scopus rating (2001): SJR 0.966 SNIP 1.284
High Pressure Rheological Behavior of 1-Ethyl-3-methylimidazolium n-Hexylsulfate and Trihexyl(tetradecyl)phosphonium Tris(pentafluoroethyl)trifluorophosphate

Ionic liquids have been broadly studied in the past decade for being used as lubricants or lubricant additives. The rheological characterization of these fluids is very important in this context because it determines to a great extent their performance for different lubricants applications, such as hydraulic or gear lubricants. Thus, in this work we have performed the rheometric characterization of two ionic liquids (ILs), 1-ethyl-3-methylimidazolium n-hexylsulfate and trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate, in the temperature range from 298.15 to 353.15 K up to 75 MPa and shear rates up to 1000 s⁻¹. For this aim, the setup of a new device for rheological characterization at high pressure based on Couette flow and concentric cylinders was undertaken in this work. Moreover the pressure–viscosity and temperature–viscosity coefficients of these ILs have been calculated. Both ILs present Newtonian behavior in the studied conditions. The trifluorophosphate IL has strong pressure–viscosity dependence, whereas for the other IL this dependence is quite slight.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, University of Santiago de Compostela, University of Vigo
Authors: Regueira, T. (Intern), Lugo, L. (Ekstern), Comuñas, M. J. P. (Ekstern), Fernández, J. (Ekstern)
Pages: 2927-2936
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 62
Issue number: 9
ISSN (Print): 0021-9568
Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
High-resolution absorption measurements of NH\textsubscript{3} at high temperatures: 2100–5500 cm\textsuperscript{-1}

High-resolution absorption spectra of NH\textsubscript{3} in the region 2100–5500 cm\textsuperscript{-1} at 1027 °C and approximately atmospheric pressure (1045±3 mbar) are measured. An NH\textsubscript{3} concentration of 10% in volume fraction is used in the measurements. Spectra are recorded in a high-temperature gas-flow cell using a Fourier Transform Infrared (FTIR) spectrometer at a nominal resolution of 0.09 cm\textsuperscript{-1}. The spectra are analysed by comparison to a variational line list, BYTe, and experimental energy levels determined using the MARVEL procedure. 2308 lines have been assigned to 45 different bands, of which 1755 and 15 have been assigned or observed for the first time in this work.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University College London
Authors: Barton, E. J. (Ekstern), Yurchenko, S. N. (Ekstern), Tennyson, J. (Ekstern), Clausen, S. (Intern), Fateev, A. (Intern)
Number of pages: 6
Pages: 60-65
Publication date: 2017
Main Research Area: Technical/natural sciences
High Temperature Heat Pump Integration using Zeotropic Working Fluids for Spray Drying Facilities

This paper presents an analysis of high temperature heat pumps in the industrial sector and demonstrates the approach of using zeotropic mixtures to enhance the overall efficiency. Many energy intensive processes in industry, such as drying processes, require heat at a temperature above 100 °C and show a large potential to reuse the excess heat from exhaust gases. This study analyses a heat pump application with an improved integration by choosing the working fluid as a mixture in such a way, that the temperature glide during evaporation and condensation matches the temperature glide of the heat source and sink best possibly. Therefore, a set of six common working fluids is defined and the possible binary mixtures of these fluids are analyzed. The performance of the fluids is evaluated based on the energetic performance...
(COP) and the economic potential (NPV). The results show that the utilization of mixtures allows a heat pump application to preheat the drying air to 120 °C with a COP of 3.04 and a NPV of 0.997 Mio. €, which could reduce the natural gas consumption by 36 %.

General information
State: Published
Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Zühlsdorf, B. (Intern), Bühler, F. (Intern), Mancini, R. (Intern), Cignitti, S. (Intern), Elmegaard, B. (Intern)
Number of pages: 11
Publication date: 2017

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Title of host publication: Proceedings of the 12th IEA Heat Pump Conference 2017
Main Research Area: Technical/natural sciences
Conference: 12th IEA Heat Pump Conference, Rotterdam, Netherlands, 15/05/2017 - 15/05/2017
Heat Pump Integration, Zeotropic Mixtures, Spray Dryer, Industrial Sector, Industrial Heat Pumps
Electronic versions:
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Relations
Projects:
High Temperature Heat Pump Integration using Zeotropic Working Fluids for Spray Drying Facilities
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Homology to peptide pattern for annotation of carbohydrate-active enzymes and prediction of function
Background: Carbohydrate-active enzymes are found in all organisms and participate in key biological processes. These enzymes are classified in 274 families in the CAZy database but the sequence diversity within each family makes it a major task to identify new family members and to provide basis for prediction of enzyme function. A fastand reliable method for de novo annotation of genes encoding carbohydrate-active enzymes is to identify conserved peptides in the curated enzyme families followed by matching of the conserved peptides to the sequence of interest as demonstrated for the glycosyl hydrolase and the lytic polysaccharide monooxygenase families. This approach not only assigns the enzymes to families but also provides functional prediction of the enzymes with high accuracy.

Results: We identified conserved peptides for all enzyme families in the CAZy database with Peptide Pattern Recognition. The conserved peptides were matched to protein sequence for de novo annotation and functional prediction of carbohydrate-active enzymes with the Hotpep method. Annotation of protein sequences from 12 bacterial and 16 fungal genomes to families with Hotpep had an accuracy of 0.84 (measured as F1-score) compared to semiautomatic annotation by the CAZy database whereas the dbCAN HMM-based method had an accuracy of 0.77 with optimized parameters. Furthermore, Hotpep provided a functional prediction with 86% accuracy for the annotated genes. Hotpep is available as a stand-alone application for MS Windows.

Conclusions: Hotpep is a state-of-the-art method for automatic annotation and functional prediction of carbohydrate-active enzymes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Busk, P. K. (Intern), Pilgaard, B. (Intern), Lezyk, M. J. (Intern), Meyer, A. S. (Intern), Lange, L. (Intern)
Number of pages: 9
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: B M C Bioinformatics
Volume: 18
Article number: 214
ISSN (Print): 1471-2105
Ratings:
BFI (2018): BFI-level 1
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.54 SJR 1.467 SNIP 0.946
Fast pyrolysis of biomass produces a high yield of bio-oil through well-established technologies [1]. To utilize this oil as liquid fuel the oxygen content must be reduced from 15-30 wt.% down to <1 wt.%, which increases heating value and stability and decreases acidity [1]. Upgrading bio-oil by catalytic hydrodeoxygenation (HDO) is challenged by severe polymerization and coking upon heating the oil. Alternatively, performing fast pyrolysis in high-pressure hydrogen atmosphere in a fluid bed reactor with a HDO catalyst as bed medium, could immediately stabilize reactive pyrolysis vapors [2]. An additional vapor phase HDO reactor could ensure removal of oxygen down to <1 wt%, resulting in separate hydrocarbon oil and water phases being recovered. A schematic diagram for such a process is shown in Figure 1. A simplified bench scale setup of this process has been constructed at DTU Chemical Engineering. With a capacity of 100 to 300 g/h solid biomass, the aim is to provide a proof-of-concept for the continuous conversion of solid biomass to low oxygen, fuel-grade bio-oil.
Hvornår bryder en kunstig muskel sammen? Simulering af termiske sammenbrud i dielektriske elastomerer

Dielektriske elastomerer kan blandt andet bruges til kunstige muskler, højttalere og til at udvinde energi fra havbølger. Ved brug af dielektriske elastomerer genereres varme grundet den elektriske modstand i materialet, hvilket kan lede til, at materialet bryder sammen. Tre essentielle parametre påvirker sammenbruddet af dielektriske elastomerer.

**General information**

**State:** Published

**Organisations:** Department of Chemical and Biochemical Engineering, The Danish Polymer Centre

**Authors:** Madsen, L. R. (Intern), Hassager, O. (Intern), Skov, A. L. (Intern)

**Pages:** 12-15

**Publication date:** 2017

**Main Research Area:** Technical/natural sciences

**Journal:** Dansk Kemi

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- ISI indexed (2011): ISI indexed no
- Web of Science (2007): Indexed yes
- Web of Science (2004): Indexed yes

**Original language:** English

**Electronic versions:**

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**Source:** PublicationPreSubmission

**Source-ID:** 140259070

**Publication:** Communication › Journal article – Annual report year: 2017

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**Hydrogen assisted catalytic biomass pyrolysis for green fuels**

Fast pyrolysis of biomass is a well-known technology for producing bio-oil, however in order to use the oil as transportation fuel the oxygen content must be decreased from approximately 30 wt.% to below 1 wt.%. This can be achieved by catalytic hydrodeoxygenation (HDO). Unfortunately, deactivation due to coking of the catalyst is an inhibitive problem for this technology. The objective of the present work is to produce oxygen free gasoline and diesel from biomass by hydrogen assisted catalytic fast pyrolysis. Fast pyrolysis of beech wood has been performed in high-pressure hydrogen atmosphere in a fluid bed reactor with a commercial CoMoS/MgAl2O4 catalyst as bed medium followed by an additional vapor phase, fixed bed HDO reactor using a commercial NiMoS/Al2O3 catalyst. The obtained bio-oil is essentially oxygen free. Oxygen specific GC-AED showed only traces of phenols, benzofurans and naphthols (< few ppm) as the remaining oxygenates. The temperature in the fluid bed reactor has been varied between 365 and 470 °C and pressure has been varied between 15 and 35 barg in order to investigate the impact on yields and oil composition. The char yield decreased with increasing temperature and decreasing pressure. Increasing the pressure also increased the water yield and decreased the CO/CO2 yield, indicating that the reaction pathway for the oxygen removal is highly pressure dependent. GCxGC-FID analysis of the condensed oil product showed a chromatic area up to 79 % for aromatics, indicating that the aromatic content in the oil is equilibrium controlled. Elemental analysis showed that the oxygen content in the char decreased with increasing temperature in the fluid bed reactor. Oil yields of up to 21.6 wt.% were obtained, corresponding to an energy recovery of 51 %. An experiment without the HDO reactor showed that most oxygen is removed in the fluid bed reactor.

**General information**
Hydrogen assisted catalytic biomass pyrolysis for green fuels

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Haldor Topsoe AS
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Event: Abstract from TCbiomass 2017, Chicago, United States.
Main Research Area: Technical/natural sciences
Electronic versions: TCbiomass2017v5.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Imaging for monitoring downstream processing of fermentation broths

In relation to downstream processing of a fermentation broth coagulation/flocculation is a typical pretreatment method for separating undesirable particles/impurities from the wanted product. In the coagulation process the negatively charged impurities are destabilized by adding of a clarifying agent thereby neutralizing the charges on the particles. Particles thus agglomerate. Larger agglomerates are formed in the flocculation process by adding a polymer, which forms bridges between the particles. The operation of coagulators, flocculators and clarifiers requires trained operators implying the human factor to play a major risk with regard to performance. Better process monitoring will provide the means for improved control giving higher yield, better quality, and minimize the consumption of water. In particular, the optimal separation of biomass from a soluble enzyme phase is often dependent on an initial coagulation of the biomass and a final flocculation of the solids just prior to separation. We investigate flocculation processes at Novozymes facilities so that the response time and risk of error is minimized. We use oCelloScope [1], an automated microscope, for imaging samples from the flocculation process and subsequently we extract image features for qualitative and quantitative image characterization. The processing include image morphology, image segmentation and image quantification. The aim is to correlate image information to “quality” of the separation process. Here we report our initial finding. [1] M.Fredborg et al. Journal of Clinical Microbiology Vol 51 Number 7 p. 2047–2053 (2013); http://www.biosensesolutions.dk

**General information**
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Statistics and Data Analysis, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Novozymes A/S, ParticleTech
Authors: Moiseyenko, R. (Intern), Baum, A. (Intern), Jørgensen, T. M. (Intern), Gianville, S. (Ekstern), Laursen, C. N. (Ekstern), Mansouri, S. S. (Intern), Gernaey, K. V. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from Recent Advances in Fermentation Technology (RAFT 2017), Florida, United States.
Main Research Area: Technical/natural sciences
Electronic versions: P46.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017
Imaging of Flames in Cement Kilns To Study the Influence of Different Fuel Types

The cement industry aims to use an increased amount of alternative fuels to reduce production costs and CO2 emissions. In this study three cement plants firing different kinds and percentages of alternative fuel were studied. A specially developed camera setup was used to monitor the flames in the three cement kilns and assess the effect of alternative fuels on the flame. It was found that cofiring with solid recovered fuel (SRF) would delay the ignition point by about 2 m and lower the intensity and temperature of the kiln flame compared to a fossil fuel flame. This is related to a larger particle size and moisture content of the alternative fuels, which lowers the conversion rate compared to fossil fuels. The consequences can be a lower kiln temperature and cement quality. The longer conversion time may also lead to the possibility of localized reducing conditions in the cement kiln, which can have a negative impact on the clinker quality and process stability. The burner design may alleviate some of the issues encountered with SRF cofiring. At one of the test plants the burner was changed from a design with an annular channel for axial air to a jet design. This proved to be beneficial for an early ignition and improved dispersion of the fuel and led to an increase in cement quality and higher use of SRF.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), F.L. Smith A/S
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Main Research Area: Technical/natural sciences

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Journal: Energy and Fuels
Volume: 31
Issue number: 10
ISSN (Print): 0887-0624
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.05
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
Impact of KCl impregnation on single particle combustion of wood and torrefied wood

In this work, single particle combustion of raw and torrefied 4 mm wood particles with different potassium content obtained by KCl impregnation and washing was studied experimentally under a condition of 1225 °C, 3.1% O₂ and 26.1% H₂O. The ignition time and devolatilization time depended almost linearly on the fuel particle mass. The char conversion time was influenced by both the char mass and char reactivity. Both KCl impregnation and torrefaction promoted char yield, while washing slightly inhibited char formation. The char reactivity was increased by KCl impregnation, decreased by washing, and unchanged by torrefaction. Compared to the raw wood particle, the char conversion time was increased by torrefaction, decreased by washing, and almost unchanged by KCl impregnation due to its promoting effect on both char yield and reactivity.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, South China University of Technology
Pages: 684-689
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.9 SJR 1.744 SNIP 2.179
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.809 SNIP 2.125 CiteScore 4.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.667 SNIP 2.331 CiteScore 4.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.811 SNIP 2.595 CiteScore 4.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
In order to maximize enzymatic xylan depolymerization while simultaneously purifying the resulting monosaccharide (xylose), different ultrafiltration (UF) membrane reactor configurations were evaluated. Initial results showed that the two hydrolytic enzymes required for complete depolymerization of xylan, endo-1,4-β-xylanase and β-xylosidase, promoted different types of fouling, which had a direct impact on the extent of xylan hydrolysis achieved during reaction. Endo-1,4-β-xylanase generated DP 1-6 xylo-oligomers. These products contributed to partial pore blocking of the 1 kDa polysulfone membrane and caused irreversible flux loss (∼20%). The presence of β-xylosidase could not prevent deposition of xylan and xylooligosaccharides on the UF membrane surface. Mulder’s modelling of the filtration parameters affirmed that this xylan and xylooligosaccharide deposition formed a cake layer on the membrane which hindered enzymatic attack in addition to fouling. Reaction with both enzymes followed by UF was found to be the optimal configuration, providing at least 40% higher xylan hydrolysis than the cascade configuration (involving sequential reaction with each of the enzymes separately) and the simultaneous reaction-filtration with both enzymes, respectively. This study thus confirmed that the reactor configuration has a crucial impact on the performance of both the reaction and the separation process of xylose during enzymatic xylan degradation, and that the type of fouling mechanism varies in response to the type of enzyme treatment.
Implementation of advanced process control on the four tank pilot plant
The four tank process laboratory experiment is used as a relevant case to unfold problems that arise when implementing advanced process control such as model predictive control. The controller, which is executed on a computer, and the process equipment communicate using OPC to exchange process measurements and actuator set points. The process equipment is described along with the setup of the PLC and the OPC server in order to be able to access process variables on a dimensional scale. A process emulator in which a process simulator is embedded in an OPC interface has been developed in Python. Using the detailed information of sensor and actuator calibration as well as PLC functionality, the emulator appears identical to the actual process and may be used to perform virtual tests of controllers prior to commissioning. Examples of how to interact with OPC servers are presented for both Matlab and Python. An MPC has been designed based on a linearized model of the process and tested using the emulator. This controller was then implemented on a realization of the process at the Technical University of Denmark, demonstrating MPC experimentally.

General information
State: Published
Organisations: Centre for IT-Intelligent Energy Systems in Cities, Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Schroll-Fleischer, E. (Intern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
Number of pages: 114
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Publisher: Technical University of Denmark (DTU)
Original language: English
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Publication: Research › Report – Annual report year: 2017

Implementation of the resource recovery concept in the biotech industry
The concept of circular economy is attracting significant attention in modern biotech industry. Downstream processing plants are usually focused on the removal of impurities instead of their recovery in the form of value-added products for additional revenues. For example, carboxylic acids, carbohydrates, proteins, lipids, inorganic ions and water itself are amongst various resources that are found in wastewater streams coming from bio-based production processes. Such compounds have a high value at the global market and could potentially be used as raw materials for the manufacturing feed and food additives, cosmetics, medical products, bio-based plastics, bio-fuels (biogas, bioethanol and biodiesel), fertilizers, and even biopharmaceuticals.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre
Authors: Mitic, A. (Intern), Mansouri, S. S. (Intern), S.B.A. Udugama, I. (Intern), Gernaey, K. V. (Intern)
Number of pages: 2
Publication date: 2017
Event: Abstract from 10th World Congress of Chemical Engineering (WCCE10), Barcelona, Spain.
Main Research Area: Technical/natural sciences
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Importance of soil NO emissions for the total atmospheric NOx budget of Saxony, Germany

Soils are a significant source for the secondary greenhouse gas NO and assumed to be a significant source of tropospheric NOx in rural areas. Here we tested the LandscapeDNDC model for its capability to simulate magnitudes and dynamics of soil NO emissions for 22 sites differing in land use (arable, grassland and forest) and edaphic as well as climatic conditions. Overall, LandscapeDNDC simulated mean soil NO emissions agreed well with observations ($r^2 = 0.82$). However, simulated day to day variations of NO did only agree weakly with high temporal resolution measurements, though agreement between simulations and measurements significantly increased if data were aggregated to weekly, monthly and seasonal time scales. The model reproduced NO emissions from high and low emitting sites, and responded to fertilization (mineral and organic) events with pulse emissions. After evaluation, we linked the LandscapeDNDC model to a GIS database holding spatially explicit data on climate, land use, soil and management to quantify the contribution of soil biogenic NO emissions to the total NOx budget for the State of Saxony, Germany. Our calculations show that soils of both agricultural and forest systems are significant sources and contribute to about 8% (uncertainty range: 6–13%) to the total annual tropospheric NOx budget for Saxony. However, the contributions of soil NO emission to total tropospheric NOx showed a high spatial variability and in some rural regions such as the Ore Mts., simulated soil NO emissions were by far more important than anthropogenic sources.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Risø National Laboratory for Sustainable Energy, Karlsruhe Institute of Technology KIT, Universitat Stuttgart, Competence Centre Wood and Forestry, INRA Institut National de La Recherche Agronomique, Agroscope Research Station, Hungarian Meteorological Service, European Commission Joint Research Centre Institute, Vrije Universiteit, International Livestock Research Institute

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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
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Web of Science (2015): Indexed yes
Scopus rating (2016): CiteScore 4.01 SJR 1.466 SNIP 1.593
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Scopus rating (2015): SJR 1.759 SNIP 1.597 CiteScore 3.73
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.593 SNIP 1.67 CiteScore 3.55
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.753 SNIP 1.63 CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.968 SNIP 1.699 CiteScore 3.47
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.982 SNIP 1.78 CiteScore 3.84
Hydrogen isocyanide (HNC) has been proposed as an important intermediate in oxidation of hydrogen cyanide (HCN) in combustion, but details of its chemistry are still in discussion. At higher temperatures, HCN and HNC equilibrate rapidly, and being more reactive than HCN, HNC offers a fast alternative route of oxidation for cyanides. However, in previous modeling, it has been required to omit the HNC subset partly or fully in the reaction mechanisms to obtain satisfactory predictions. In the present work, we re-examine the chemistry of HNC and its role in combustion nitrogen chemistry. The HNC + O2 reaction is studied by ab initio methods and is shown to have a high barrier. Consequently, the omission of this reaction in recent modeling studies is justified. With the present knowledge of the HNC chemistry, including an accurate value of the heat of formation for HNC and improved rate constants for HNC + O2 and HNC + OH, it is possible to reconcile the modeling issues and provide a satisfactory prediction of a wide range of experimental results on HCN oxidation. In the burned gases of fuel-rich flames, HCN and the CN radical are partially equilibrated and the sequence HCN → +M HNC → +OH HNCO is the major consumption path for HCN. Under lean conditions, HNC is shown to be less important than indicated by the early work by Lin and co-workers, but it acts to accelerate HCN oxidation and promotes the formation of HNCO.
Improvement of predictive tools for vapor-liquid equilibrium based on group contribution methods applied to lipid technology

Predictive methodologies based on group contribution methods, such as UNIFAC, play a very important role in the design, analysis and optimization of separation processes found in oils, fats and biodiesel industries. However, the UNIFAC model
has well-known limitations for complex molecular structures that the first-order functional groups are unable to handle. In the particular case of fatty systems these models are not able to adequately predict the non-ideality in the liquid phase. Consequently, a new set of functional groups is proposed to represent the lipid compounds, requiring thereby, new group interaction parameters. In this work, the performance of several UNIFAC variants, the Original-UNIFAC, the Linear-UNIFAC, Modified-UNIFAC and the Dortmund-UNIFAC is compared. The same set of experimental data and the parameter estimation method developed by Perederic et al. (2017) have been used. The database of measured data comes from a special lipids database developed in-house (SPEED Lipids database at KT-consortium, DTU, Denmark). All UNIFAC models using the new lipid-based parameters show, on average, improvements compared to the same models with their published parameters. There are rather small differences between the models and no single model is the best in all cases.

General information
State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CERE – Center for Energy Resources Engineering, Technical University of Denmark, University of Campinas
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Publication date: 2017
Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Improving efficiency of heat pumps by use of zeotropic mixtures for different temperature glides

The present study demonstrates the optimization of a heat pump for an application with a large temperature glide on the sink and a smaller temperature glide on the source side. The study includes a simulation of a heat pump cycle for all possible binary mixtures from a list of 14 natural refrigerants, which enables a match of the temperature glide of sink and source with the temperature of the working fluid during phase change and thus, a reduction of the exergy destruction due to heat transfer. The model was evaluated for four different boundary conditions. For a separated evaluation of the irreversibility solely caused by the fluid properties, the exergy destruction in the heat exchangers has been distinguished accordingly and an indicator quantifying the glide match has been defined to analyse the influence on the performance. It was observed that a good glide match can contribute to an increased performance. Dependent on the boundary conditions a performance increase of 20.0 % for a simple cycle was observed and 26.9 % increase if the required superheating can be avoided. The temperature glide match in the source was identified to have a higher influence on the performance than in the sink.

General information
State: Published
Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Danish Technological Institute
Authors: Zühlsdorf, B. (Intern), Jensen, J. K. (Intern), Cignitti, S. (Intern), Madsen, C. (Ekstern), Elmegaard, B. (Intern)
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Main Research Area: Technical/natural sciences
Conference: 30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, San Diego, United States, 02/07/2017 - 02/07/2017
Heat pump, Zeotropic mixture, Temperature glide, Exergy efficiency

Relations
**Improving the Prediction of Phosphate Dynamics in Biotechnological Processes: A Case Study Based on Antibiotic Production Using *Streptomyces coelicolor***

The objective of this study is to demonstrate that the accurate mathematical description of phosphate dynamics requires a considerable, but unavoidable, degree of complexity when modelling biotechnological systems. As an example, a model predicting antibiotic production using *Streptomyces coelicolor* is chosen which had difficulties explaining the phosphate dynamics. The model is enhanced by the implementation of an advanced speciation model and a multiple mineral precipitation framework. Furthermore, a model describing intracellular polyphosphate accumulation and consumption is developed and implemented. Based on the conducted work the improved process model is capable of predicting the phosphate dynamics (RMSE< 52h: -90 %, RAD< 52h: -96 %) very accurately in comparison to the original implementation, where biomass growth was the only phosphate sink. The description of most other variables was improved by a knowledge-based re-estimation of selected parameters as well. This work contributes to the existing process knowledge of biotechnological systems in general and especially to the antibiotic production with *S. coelicolor*, which emphasizes the necessity of combining physico-chemical and biological processes to accurately describe phosphate dynamics.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Brandenburg University of Technology, University of Surrey  
Authors: Bürger, P. (Ekstern), Flores-Alsina, X. (Intern), Arellano-Garcia, H. (Ekstern)  
Pages: 2869-2874  
Publication date: 2017

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Title of host publication: *Proceedings of the 27th European Symposium on Computer Aided Process Engineering – ESCAPE 27*

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Series: Computer - Aided Chemical Engineering  
ISSN: 1570-7946  
Main Research Area: Technical/natural sciences  
Conference: 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 01/10/2017 - 01/10/2017  
Streptomyces coelicolor, Process modelling, Speciation, Precipitation, Polyphosphate  
DOIs: 10.1016/B978-0-444-63965-3.50480-3

Industri al Coatings at Extreme Conditions

With the gradual depletion of oil wells operable at relatively lower temperatures and pressures, the upstream oil industry relies on High Pressure High Temperature (HPHT) wells to source crude oil and gas. HPHT well extraction and processing require anticorrosive coatings applied on substrates such as downhole piping and pressure vessels that can withstand such temperature and pressures. Very little information is available regarding the degradation mechanisms of currently used solvent-borne epoxy coatings in these conditions. Cyclic stress tests at lower temperatures (25-85 °C) [I] resulted in coating fractures and holes from collapsed blisters originating from thermal shocks.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Technical University of Denmark, Hempel AS  
Authors: Subramanian, S. (Ekstern), Pérez Hornero, C. (Ekstern), Pedersen, L. T. (Ekstern), Kiil, S. (Intern)  
Number of pages: 3  
Publication date: 2017  
Main Research Area: Technical/natural sciences  
Electronic versions: Srinath_Subramaninan_COSI_2017.pdf

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Influence of extensional stress overshoot on crystallization of LDPE

Low-density polyethylene (LDPE) shows a stress overshoot in start-up of strong uniaxial extensional flows of constant rate. It is believed that the overshoot is caused by a contraction of the polymer backbone due to alignment of the long chain branches, the consequence being that the molecular strain of the backbone does not increase monotonically with the global strain of the melt. In this study we investigate the semicrystalline morphology of LDPE quenched before, after, and at the overshoot. We do this by combining filament stretching rheometry with ex-situ X-ray scattering. It is found that the overshoot indeed is reflected in the orientation of the crystalline domains of the quenched filaments. In a broader perspective, we show that the final crystalline morphology is determined by the stress at quench rather than the strain at quench. With these findings we confirm that the much debated overshoot has a physical origin. More importantly, we conclude that even for complex architectures like branched systems, the crystalline orientation is determined by the backbone stretch rather than the global stretch of the material.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, University of Nottingham, University of Copenhagen
Authors: Wingstrand, S. L. (Intern), van Drongelen, M. (Intern), Mortensen, K. (Ekstern), S. Graham, R. (Ekstern), Huang, Q. (Intern), Hassager, O. (Intern)
Pages: 1134–1140
Publication date: 2017
Main Research Area: Technical/natural sciences
Influence of fungal morphology on the performance of industrial fermentation processes for enzyme production

Production of industrial enzymes is usually carried out as submerged aerobic fermentations. Filamentous microorganisms are widely used as hosts in these processes due to multiple advantages. Nevertheless, they also present major drawbacks, due to the unavoidable oxygen transfer limitations as a consequence of the high viscosity of the medium that they develop, which is believed to be related to the biomass concentration, growth rate and morphology. This last variable is one of the most outstanding characteristics of the filamentous fungi due to its great complexity and it was extensively studied in this work, along with its correlation to viscosity and other process variables. Considerable research work has been conducted through the years to study fungal morphology and its relation to productivity. However, the work reported in the literature lacks relevant industrial data. In this work, a platform was developed which was able to produce high enzyme titers in comparison with what has been reported thus far in fed-batch fermentation using a soluble inducer (lactose). Different nitrogen sources were compared, and it was found that soy meal allowed for higher enzyme titers compared to what has been reported in the literature.

The developed platform was used to study the influence of agitation intensity on the morphology, rheology and protein production capability of Trichoderma reesei RUT-C30. Eight fed-batch fermentations were conducted in bench scale fermenters at two different media concentrations and four different agitation speeds. The morphology was measured with laser diffraction and the 90th percentile of the particle size distribution (PSD) was chosen as the characteristic morphology parameter. No significant difference in biomass concentration, carbon dioxide production rate and enzyme production was observed as a function of agitation speed, even at the very high power inputs. However, the morphology and rheology were considerably affected. The data produced was used to create a novel method to predict filamentous fungi rheology based on simple measurements of biomass and morphology.

Thus, morphology is an important variable in industrial submerged fermentation since it highly impacts the broth rheology. Therefore, it is important to understand the factors that affect it. One important factor is agitation-induced fragmentation since it will dictate the size of the particles, which will then affect rheology. A well-established state of the art function, the Energy Dissipation Circulation Function (EDCF), has been used to correlate hyphal fragmentation over a range of scales and impeller types. This correlation was however developed for non-growing systems (off-line fragmentation), and no attempts have been made for testing its application across different scales in actual fermentation broths. To test the validity of this correlation, a scale-down experiment was carried out. A production batch from Novozymes A/S operated in a production scale bioreactor (~100 m\(^3\)) was scaled down to pilot scale (~1 m\(^3\)) and to bench scale (~0.001 m\(^3\)). The EDCF was calculated for each batch along with other mixing parameters and they were correlated to the characteristic morphological parameter, the 90th percentile of the PSD. The data showed that other more simple scale up parameters are equally good at predicting mycelial fragmentation across scales, compared to the EDCF.

Furthermore, the morphological development of an industrial strain of T. reesei was monitored in pilot scale fermentations. This study showed that the morphology monitored with laser diffraction also granted the possibility to study direct physiological responses to environmental conditions in stirred bioreactors. The obtained results indicate that the nutrient
depletion induced foraging due to starvation, which caused the increase in hyphal length. Finally, a novel, fast and easy method for statistically-verified quantification of relative hyphal tensile strength was developed in the last part of this PhD project. Fungal hyphal strength is an important phenotype which can have a profound impact on bioprocess behavior. The applicability of this novel method was demonstrated by estimating relative hyphal strength during growth in control conditions and rapamycin-induced autophagy conditions for two strains of Aspergillus nidulans. Both strains were grown in shake flasks, and relative hyphal tensile strength was compared. The findings confirmed the utility of the developed method in strain selection and process development. This PhD thesis brings more knowledge to the understanding of the relationship between growth kinetics, environmental conditions and the morphological structure of the filamentous fungi, which can help to tailor the morphology for a given industrial strain.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, The Danish Polymer Centre, PILOT PLANT, Novozymes A/S
Authors: Quintanilla Hernandez, D. A. (Intern), Gernaey, K. (Intern), Hassager, O. (Intern), Eliasson Lantz, A. (Intern), Hansen, K. (Ekstern)
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Relations
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Influence of fungal morphology on the performance of industrial fermentation processes for enzyme production
Publication: Research › Ph.D. thesis – Annual report year: 2017

Influence of preoxidation on high temperature corrosion of a Ni-based alloy under conditions relevant to biomass firing
Development of corrosion resistant materials in biomass fired power plants demands specific attention since the condensation of deposits rich in KCl on heat exchanger surfaces induces severe corrosion attack, which is different from corrosion in traditional coal fired plants. Therefore, the ability of preoxidized layers formed on a commercial Cr-Ti-Al-containing Ni-based alloy (Nimonic 80A) to withstand biomass-induced corrosion was investigated. Preoxidation treatments at 900 °C in O2 and O2 + 10 vol% H2O, respectively, were conducted before samples were exposed to conditions that mimicked biomass firing. Complementary characterization methods were employed to study samples after preoxidation as well as after corrosion exposure. The oxides obtained by the preoxidation treatments protected the alloy during corrosion exposure at 560 °C for a period of 168 h. In contrast, non-preoxidized samples suffered corrosion attack and formed porous non-protective oxides containing the alloying elements, Ni, Cr, Ti and Al. The influence of the preoxidation layers on the corrosion mechanism is discussed.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Mechanical Engineering, Materials and Surface Engineering
Authors: Okoro, S. C. (Intern), Montgomery, M. (Intern), Jappe Frandsen, F. (Intern), Pantleon, K. (Intern)
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Influence of Promotor, H₂O and H₂S on the Hydrodeoxygenation of Biomass Pyrolysis Vapor over MoS₂ Catalysts

Catalytic hydropyrolysis combines fast pyrolysis with catalytic upgrading by hydrodeoxygenation (HDO) in a single step for the production of fuel oil from biomass in which reactive pyrolysis vapors are upgraded before condensation. Catalyst activity and lifetime is challenged by carbon deposition and by the presence of alkali, nitrogen, sulfur and water. In this contribution, a combined experimental, characterization (in-situ Extended X-Ray Absorption Fine Structure, EXAFS) and...
A theoretical (Density Functional Theory, DFT) study of catalytic HDO of biomass model compounds over MoS\(_2\) based catalysts is presented with emphasis on the influence of water and H\(_2\)S.

### General information
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Karlsruhe Institute of Technology KIT, Stanford University, Haldor Topsoe AS, Technical University of Denmark
- **Authors:** Arndal, T. M. H. (Intern), Høj, M. (Intern), Gaur, A. (Ekstern), Früssmann, T. (Ekstern), Pintos, D. G. (Ekstern), Studt, F. (Ekstern), Gabrielsen, J. (Ekstern), Grunwaldt, J. (Ekstern), W. Hansen, T. (Ekstern), Jensen, A. D. (Intern)
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### Influence of Promotor, H\(_2\)O and H\(_2\)S on the Hydrodeoxygenation of Biomass Pyrolysis Vapor over MoS\(_2\) Catalysts

Catalytic hydropyrolysis combines fast pyrolysis with catalytic upgrading by hydrodeoxygenation (HDO) in a single step for the production of fuel oil from biomass in which reactive pyrolysis vapors are upgraded before condensation. Catalyst activity and lifetime is challenged by carbon deposition and by the presence of alkali, nitrogen, sulfur and water. In this contribution, a combined experimental, characterization (in-situ Quick-EXAFS) and theoretical (DFT) study of catalytic HDO of biomass pyrolysis model compounds over MoS2 based catalysts is presented with emphasis on the influence of water and H2S.

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- **Authors:** Arndal, T. M. H. (Intern), Høj, M. (Intern), Gaur, A. (Ekstern), Früssmann, T. (Ekstern), Pintos, D. G. (Ekstern), Studt, F. (Ekstern), Gabrielsen, J. (Ekstern), Grunwaldt, J. (Ekstern), W. Hansen, T. (Ekstern), Jensen, A. D. (Intern)
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### Influence of temperature and solvent concentration on the kinetics of the enzyme carbonic anhydrase in carbon capture technology

In this study the effect of carbonic anhydrase addition on the absorption of CO\(_2\) was investigated in a wetted wall column apparatus. Four different solvents: the primary amine monoethanolamine (MEA), the sterically hindered primary amine 2-amino-2-methyl-1-propanol (AMP), the tertiary amine N-methyl-diethanolamine (MDEA) and the carbonate salt solution K\(_2\)CO\(_3\) were compared in concentrations from 5 to 50 wt% in a temperature range of 298–328 K with and without enzyme. Necessary mass transfer parameters such as liquid side mass transfer coefficient and solvent and enzyme reaction rates were determined and benchmarked to a 30 wt% MEA solution. The study reveals that the addition of the enzyme carbonic anhydrase (CA) dramatically increases the liquid side mass transfer coefficient for MDEA and K\(_2\)CO\(_3\); AMP has a moderate increase whereas MEA was unchanged. The results confirm that just bicarbonate forming systems benefit from CA. The influence of temperature on the enzyme kinetics and mass transfer coefficients is different for different solvent types. A temperature increase resulted in lower liquid side mass transfer coefficient for MDEA and K\(_2\)CO\(_3\) but in a higher coefficient for AMP. The overall first order enzyme reaction rate (s\(^{-1}\)) was linearly dependent on enzyme concentration for MDEA and K\(_2\)CO\(_3\) at 313 K. Temperature and concentration did increase the enzymatic rate constant slightly in the concentration range of 5–15 wt% K\(_2\)CO\(_3\) and significantly between 15 and 20 wt%. The enzymatic reaction rate constant for MDEA decreased with temperature, the solvent concentration had a negligible on it. The enzymatic reaction rate for AMP rose with temperature and was higher for lower solvent concentration.

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- **Organisations:** Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS
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- **Pages:** 772-786
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In-situ hydrodeoxygenation of phenol by supported Ni catalyst-explanation for catalyst performance

In-situ hydrodeoxygenation of phenol with aqueous hydrogen donor over supported Ni catalyst was investigated. The supported Ni catalysts exerted very poor performance, if formic acid was used as the hydrogen donor. Catalyst modification by loading K, Na, Mg or La salt could not make the catalyst performance improved. If gaseous hydrogen was used as the hydrogen source the activity of Ni/Al₂O₃ was pretty high. CO₂ was found poisonous to the catalysis, due to the competitive adoption of phenol with CO₂. If formic acid was replaced by methanol, the catalyst performance improved remarkably, with major products of cyclohexanone and cyclohexanol. The better effect of methanol enlightened the application of the supported Ni catalyst in in-situ hydrodeoxygenation of phenol.
Insulin fibrillation: The influence and coordination of Zn$^{2+}$

Protein amyloid fibrillation is obtaining much focus because it is connected with amyloid-related human diseases such as Alzheimer's disease, diabetes mellitus type 2, or Parkinson's disease. The influence of metal ions on the fibrillation process and whether it is implemented in the amyloid fibrils has been debated for some years. We have therefore investigated the influence and binding geometry of zinc in fibrillated insulin using extended X-ray absorption fine-structure and X-ray absorption near-edge structure spectroscopy. The results were validated with fibre diffraction, Transmission Electron Microscopy and Thioflavin T fluorescence measurements. It is well-known that Zn$^{2+}$ ions coordinate and stabilize the hexameric forms of insulin. However, this study is the first to show that zinc indeed binds to the insulin fibrils. Furthermore, zinc influences the kinetics and the morphology of the fibrils. It also shows that zinc coordinates to histidine residues in an environment, which is similar to the coordination seen in the insulin $R_6$ hexamers, where three histidine residues and a chloride ion is coordinating the zinc.

**General information**

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Organisations: Department of Chemistry, X-ray Crystallography, Department of Chemical and Biochemical Engineering, The Hempel Foundation Coatings Science and Technology Centre (CoaST), University of Copenhagen, CMCassist ApS
Authors: Frankær, C. G. (Intern), Sønderby, P. (Intern), Bang, M. B. (Intern), Mateiu, R. V. (Intern), Groenning, M. (Ekstern), Bukrinski, J. (Ekstern), Harris, P. (Intern)
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Scopus rating (2014): SJR 2.496 SNIP 1.257 CiteScore 3.14
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Integrated computer-aided framework for chemical product and process application design and optimization for waste heat recovery

This contribution presents an integrated framework for product-process design. The framework integrates the two design problems into one and finds the optimal solution through simultaneous optimization. The framework consists of four hierarchical steps and uses a set of methods, tools and databases for property prediction, novel fluid design and mathematical programming. The application of the framework is targeted for waste heat recovery design systems, where the sensitivity of product and process design variables is high and the simultaneous design is necessary. The sustainable design solutions are showcased in this paper for mixed refrigeration design.

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Integrated design and sustainable assessment of innovative biomass supply chains: A case-study on miscanthus in France

Cost-efficient, environmental-friendly and socially sustainable biomass supply chains are urgently needed to achieve the 2020 targets of the Strategic Energy Technologies-Plan of the European Union. This paper investigated technical, social, economic, and environmental barriers to the development and innovation of supply chains, taking into account a large range of parameters influencing the performances of biomass systems at supply chain scale. An assessment framework was developed that combined economic optimization of a supply chain with a holistic and integrated sustainability assessment. The framework was applied to a case-study involving miscanthus biomass in the Burgundy region (Eastern France) to compare alternative biomass supply chain scenarios with different annual biomass demand, crop yield, harvest timing and densification technologies. These biomass supply chain scenarios were first economically optimized across the whole supply chain (from field to plant gate) by considering potential feedstock production (from a high-resolution map), costs, logistical constraints and product prices. Then sustainability assessment was conducted by combining recognized methodologies: economic analysis, multi-regional input-output analysis, emergy assessment, and life-cycle assessment. The analysis of the case study scenarios found that expanding biomass supply from 6,000 to 30,000 tons of dry matter per year did not impact the profitability, which remained around 20€ per ton of biomass procured. Regarding environmental impacts, the scenario with the lowest feedstock supply area had the lowest impact per ton due to low economies of scale. Mobile briquetting proved to be also a viable economic option, especially in situations with a considerable scattering of the crop production and expensive transportation logistics. By highlighting hot-spots in terms of economic, environmental and social impacts of biomass supply systems, this study provides guidance in the supply chain optimization and the design of technological solutions tailored to economic operators as well as other stakeholders, such as policy makers.
Integrated working fluid-thermodynamic cycle design of organic Rankine cycle power systems for waste heat recovery

Today, some established working fluids are being phased out due to new international regulations on the use of environmentally harmful substances. With an ever-increasing cost to resources, industry wants to converge on improved sustainability through resource recovery, and in particular waste heat recovery. In this paper, an organic Rankine cycle process and its pure working fluid are designed simultaneously for waste heat recovery of the exhaust gas from a marine diesel engine. This approach can overcome design issues caused by the high sensitivity between the fluid and cycle design variables and otherwise high resource demands, which through conventional methods cannot be addressed. The global optimal design was a 1.2 MW cycle with 2,2,3,3,4,4,5,5-octafluorohexane as the new fluid. The fluid has no ozone depletion potential and a global warming potential under the regulatory limit. By using the simultaneous design approach the optimum solution was found in 5.04 s, while a decomposed approach found the same solution in 5.77 h. However, the decomposed approach provided insights on the correlation between the fluid and cycle design variables by analyzing all possible solutions. It was shown that the high sensitivity between the fluid and cycle design variables was overcome by using the simultaneous approach. Correlation between net power output and the product of the overall heat transfer coefficient and the heat transfer area could further be addressed by employing a new solution strategy including maximum constraints for this product. The use of such constraints resulted in the design of a new fluid (5-chloro-4,5,5-trifluoro-2,3-dimethyl-pent-2-ene) with a 1.25 MW net power output. Finally, a comparison with conventional fluids was shown where 2,2,3,3,4,4,5,5-octafluorohexane offered an improvement on net power output and economic and environmental metrics.

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Authors: Cignitti, S. (Intern), Andreasen, J. G. (Intern), Haglind, F. (Intern), Woodley, J. (Intern), Abildskov, J. (Ekstern)
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Publication information
Integrating protein engineering with process design for biocatalysis

Biocatalysis uses enzymes for chemical synthesis and production, offering selective, safe and sustainable catalysis. While today the majority of applications are in the pharmaceutical sector, new opportunities are arising every day in other industry sectors, where production costs become a more important driver. In the early applications of the technology, it was necessary to design processes to match the properties of the biocatalyst. With the advent of protein engineering, organic chemists started to develop and improve enzymes to suit their needs. Likewise in industry, although not widespread, a new paradigm was already implemented several years ago to engineer enzymes to suit process needs. Today, a new era is entered, where the effectiveness with which such integrated protein and process engineering is achieved becomes critical to implementation. In this paper, the development of a tool to improve the effectiveness of this approach is discussed, namely the use of target-setting based on process requirements, to guide the necessary protein engineering.
Integration of computational modeling and experimental techniques to design fuel surrogates

Conventional gasoline comprises of a large number of hydrocarbons that makes it difficult to utilize in a model for prediction of its properties. Modeling is needed for a better understanding of the fuel flow and combustion behavior that are essential to enhance fuel quality and improve engine performance. A simplified alternative is to develop surrogate fuels that have fewer compounds and emulate certain important desired physical properties of the target fuels. Six gasoline blends were formulated through a computer aided model based technique “Mixed Integer Non-Linear Programming” (MINLP). Different target properties of the surrogate blends for example, Reid vapor pressure (RVP), dynamic viscosity (η), density (ρ), Research octane number (RON) and liquid-liquid miscibility of the surrogate blends) were calculated. In this study, more rigorous property models in a computer aided tool called Virtual Process-Product Design Laboratory (VPPD-Lab) are applied onto the defined compositions of the surrogate gasoline. The aim is to primarily verify the defined composition of gasoline by means of VPPD-Lab. ρ, η and RVP are calculated with more accuracy and constraints such as distillation curve and flash point on the blend design are also considered. A post-design experiment-based verification step is proposed to further improve and fine-tune the “best” selected gasoline blends following the computation work. Here, advanced experimental techniques are used to measure the RVP, ρ, η, RON and distillation temperatures. The experimental results are compared with the model predictions as well as the extended calculations in VPPD-Lab.
Intensification of ethylene glycol production process

This study aims to generate an alternative design for ethylene glycol production process focusing on a reduction of operating cost and emissions. To achieve this, the phenomena-based method for process intensification was applied. 3 stages of process intensification were performed. First, the base-case design was obtained, resulting in the production of ethylene glycol via two steps: ethylene oxidation synthesis followed by ethylene oxide hydration to produce ethylene glycol. Feasibility of the design was verified and the process was rigorously designed using a computer process simulation program. In the second stage, the base-case design was analysed through economic evaluation and environmental impact analysis to identify the process “hot spots” and determine targets for improvement. In the last stage, the phenomena-based method for process intensification was applied to determine more sustainable solutions. As the result of intensification method, membrane separation was suggested and applied to the design. With the operation of the new equipment, the ethylene glycol production process was improved for 54.51 percent in terms of energy consumption.

In vitro evaluation of the feed quality of enzyme treated bristles and hooves

Ethylene glycol production, Ethylene oxidation, Ethylene oxide hydration, Process intensification, Phenomena-based
Ionic Liquids for Absorption and Separation of Gases: An Extensive Database and a Systematic Screening Method

Ionic liquids (ILs) have attracted considerable attention in both the academic and industrial communities for absorbing and separating gases. However, a data-rich and well-structured systematic database has not yet been established, and screening for highly efficient ILs meeting various requirements remains a challenging task. In this study, an extensive database of estimated Henry's law constants of twelve gases in more than ten thousand ILs at 313.15 K is established using the COSMO-RS method. Based on the database, a new systematic and efficient screening method for IL selection for the absorption and separation of gases subject to important target properties is proposed. Application of the database and the screening method is highlighted through case studies involving two important gases separation problems (CO₂ from CH₄ and C₂H₂ from C₂H₄). The results demonstrate the effectiveness of using the screening method together with the database to explore and screen novel ILs meeting specific requirements for the absorption and separation of gases.

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Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Chinese Academy of Sciences
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Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
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The book Classical Thermodynamics of Fluid Systems: Principles and Applications written by professor Juan H. Vera and Dr. Grazyna Wilczek-Vera is undoubtedly a book written in a most personal style by the two distinguished authors. The book contains four sections and a fifth one with appendices (mostly on selected thermodynamic models). The first two sections contain a total of 18 chapters on fundamentals of thermodynamics and mixtures, including phase diagrams. These chapters on the fundamentals are presented in a very rigorous, mathematical and rather condensed way, in carefully formulated short chapters, with a minimum number of figures, tables, examples and references. The terminology and nomenclature is clear and consistent across the whole book. The interrelations between the thermodynamic properties and variables are presented in an exceptionally clear way and an excellent illustration of this is the equation on the cover page of Section II. Especially Chapters 14 and 15 present these interrelations of thermodynamic properties in a very comprehensive way. With the exception of Chapter 18 on electrolyte solutions, essentially no models which, as the authors say “come and go”, are presented in these first two sections. Electrolytes is an area of active research for many including the authors of the book and it is, thus, not surprising that extra attention to electrolytes is given in various places in the book, already in Section II. In addition to an entire chapter about electrolytes (Chapter 18), equilibrium involving ions is discussed in Chapter 10 and the use of molality as a measure of concentration in Chapter 15.

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Kinetics based reaction optimization of enzyme catalysed reduction of formaldehyde to methanol with synchronous cofactor regeneration

Enzymatic reduction of carbon dioxide (CO_2) to methanol (CH_3 OH) can be accomplished using a designed set-up of three oxidoreductases utilizing reduced pyridine nucleotide (NADH) as cofactor for the reducing equivalents electron supply. For this enzyme system to function efficiently a balanced regeneration of the reducing equivalents during reaction is required. Herein, we report the optimization of the enzymatic conversion of formaldehyde (CHOH) to CH3 OH by alcohol dehydrogenase, the final step of the enzymatic redox reaction of CO_2 to CH3 OH, with kinetically synchronous enzymatic cofactor regeneration using either glucose dehydrogenase (System I) or xylose dehydrogenase (System II). A mathematical model of the enzyme kinetics was employed to identify the best reaction set-up for attaining optimal cofactor recycling rate and enzyme utilization efficiency. Targeted process optimization experiments were conducted to verify the kinetically modelled results. Repetitive reaction cycles were shown to enhance the yield of CH3 OH, increase the total turnover number (TTN) and the biocatalytic productivity rate (BPR) value for both system I and II whilst minimizing the exposure of the enzymes to high concentrations of CHOH. System II was found to be superior to System I with a yield of 8 mM CH3 OH, a TTN of 160 and BPR of 24 μmol CH3 OH/U·h during 6 hours of reaction. The study demonstrates that an optimal reaction set-up could be designed from rational kinetics modelling to maximize the yield of CH3 OH, whilst simultaneously optimizing cofactor recycling and enzyme utilization efficiency. This article is protected by copyright. All rights reserved.

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Scopus rating (2010): SJR 1.538 SNIP 1.357
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BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.491 SNIP 1.356
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Scopus rating (2008): SJR 1.238 SNIP 1.288
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Web of Science (2005): Indexed yes
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Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.07 SNIP 1.177
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Kinetic study of a Layout for the Carbon Capture with Aqueous Ammonia without Salt Precipitation

This paper focuses on carbon capture in an Ultra Super Critical power plant. The technology selected for CO₂ capture is based on cooled ammonia scrubbing in post-combustion mode, as recently investigated by the authors in another work. Here, a rate-based approach is adopted. In detail, a specific primary energy consumption for CO₂ avoided (SPECCA) of 2.77 MJ/kgCO₂ is calculated in case of 85% of CO₂ capture, with an ultimate power plant efficiency of 37.27%.

Laccase catalyzed grafting of-N-OH type mediators to lignin via radical-radical coupling

Lignin is an underexploited resource in biomass refining. Laccases (EC 1.10.3.2) catalyze oxidation of phenolic hydroxyls using O₂ as electron acceptor and may facilitate lignin modification in the presence of mediators. This study assessed the reactivity of four different synthetic mediators by laccases from Trametes versicolor and Pleurotus ostreatus by quantitative analysis of the reaction outcome by pyrolysis gas chromatography mass spectroscopy. The two laccases were equally efficient in catalyzing grafting, but only-N-OH type mediators grafted. HPI (N-hydroxyacetanilide) grafted 7-10
times better than HBT (1-hydroxybenzotriazole). Three different mechanisms are suggested to explain the grafting of HPI and HBT, all involving radical-radical coupling to produce covalent bonding to lignin. Lignin from exhaustive cellulase treatment of wheat straw was more susceptible to grafting than beech organosolv lignin with the relative abundance of grafting being 35% vs. 11% for HPI and 5% vs. 1% for HBT on these lignin substrates. The data imply that lignin can be functionalized via laccase catalysis with-N-OH type mediators.
LCSoft – the Life Cycle Assessment Software: New developments and status

Life Cycle Assessment or LCA is a technique to evaluate environmental impacts through the entire life cycle of products and/or processes, which is an important key to identify the environmental hotspot and make more informed decision for process design. In order to perform LCA, LCSoft has been developed with ability to integrate with other process design tools such as process simulation software, economic analysis tool, and sustainable process design tool. In addition, several optional interpretation features are available, such as, sensitivity analysis, alternative comparison, and eco-efficiency evaluation. More specifically in this paper, LCSoft has been improved in terms of performance and application range. The development framework consists of four tasks. The first task deals with a new pathway for LCIA calculation to improve the flexibility of the software. The second task consists of extension and management options of Life Cycle Inventory database. The third task deals with development & introduction of new LCSoft features - parameter sensitivity analysis, normalization, and data quality indicator. The final task is validation of the integrated software. In this paper, assessment results for bioethanol production from cassava rhizome are compared with LCA software, SimaPro. The results indicate that the new features of LCSoft provide reliable calculations very efficiently, and are especially useful for chemical and biochemical sustainable process design studies.

Location-dependent optimal biorefinery synthesis

In this paper, we present an extended framework for synthesis of biorefinery networks. The extension of the framework responds to the needs of: automatically generating problem-specific superstructures from an in-house database in an efficient and reliable way, as well as obtaining and analysing sets of optimal and near-optimal location-dependent solutions enabling the consideration of specific criteria in the final selection. The extended framework is presented in detail, followed by an application example of ethanol production from various biomass sources. The results show the ability of the extended framework to retrieve a superstructure from the database based on a problem definition as well as to produce a set of top-ranked solutions (alternative process structures, location and feedstock selection) to be further analysed.
Low temperature circulating fluidized bed gasification and co-gasification of municipal sewage sludge. Part 1: Process performance and gas product characterization

Results from five experimental campaigns with Low Temperature Circulating Fluidized Bed (LT-CFB) gasification of straw and/or municipal sewage sludge (MSS) from three different Danish municipal waste water treatment plants in pilot and demonstration scale are analyzed and compared. The gasification process is characterized with respect to process stability, process performance and gas product characteristics. All experimental campaigns were conducted at maximum temperatures below 750°C, with air equivalence ratios around 0.12 and with pure silica sand as start-up bed material. A total of 8600kg of MSS dry matter was gasified during 133h of operation. The average thermal loads during the five experiments were 62-100% of nominal capacity. The short term stability of all campaigns was excellent, but gasification of dry MSS lead to substantial accumulation of coarse and rigid, but un-sintered, ash particles in the system. Co-gasification of MSS with sufficient amounts of cereal straw was found to be an effective way to mitigate these issues as well as eliminate thermal MSS drying requirements. Characterization of gas products and process performance showed that even though gas composition varied substantially, hot gas efficiencies of around 90% could be achieved for all MSS fuel types.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, DONG Energy Thermal Power A/S, Danish Fluid Bed Technology ApS
Authors: Thomsen, T. P. (Intern), Sárossy, Z. (Intern), Gøbel, B. (Ekstern), Stoholm, P. (Ekstern), Ahrenfeldt, J. (Intern), Jappe Frandsen, F. (Intern), Henriksen, U. B. (Intern)
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Low temperature circulating fluidized bed gasification and co-gasification of municipal sewage sludge. Part 2: Evaluation of ash materials as phosphorus fertilizer

The study is part 2 of 2 in an investigation of gasification and co-gasification of municipal sewage sludge in low temperature gasifiers. In this work, solid residuals from thermal gasification and co-gasification of municipal sewage sludge were investigated for their potential use as fertilizer. Ashes from five different low temperature circulating fluidized bed (LT-CFB) gasification campaigns including two mono-sludge campaigns, two sludge/straw mixed fuels campaigns and a straw reference campaign were compared. Experiments were conducted on two different LT-CFBs with thermal capacities of 100 kW and 6 MW, respectively. The assessment included: (i) Elemental composition and recovery of key elements and heavy metals; (ii) content of total carbon (C) and total nitrogen (N); (iii) pH; (iv) water extractability of phosphorus after incubation in soil; and (v) plant phosphorus response measured in a pot experiment with the most promising ash material. Co-gasification of straw and sludge in LT-CFB gasifiers produced ashes with a high content of recalcitrant C, phosphorus (P) and potassium (K), a low content of heavy metals (especially cadmium) and an improved plant P availability compared to the mono-sludge ashes, thereby showing the best fertilizer qualities among all assessed materials. It was also found that bottomashes from the char reactor contained even less heavy metals than cyclone ashes.

It is concluded that LT-CFB gasification and co-gasification is a highly effective way to purify and sanitize sewage sludge for subsequent use in agricultural systems.
Low Temperature DeNOx Technologies for Power and Waste Incineration Plants

Formation of NOx is inevitable during high temperature combustion processes in air. NOx is of increasing environmental concern due to its participation in detrimental photochemical reactions, which lead to ozone layer depletion. NOx emissions also cause acid rain, contribute to smog formation and induces respiratory diseases in humans. There is no doubt that anthropogenic effects are contributing to the global climate change. The largest contributor to anthropogenic greenhouse gas emissions is CO2. 

Previous work has shown that ionic liquids (ILs) are promising absorbers and can selectively absorb flue gas constituents such as CO2, SO2 and NO. Utilisation of ILs is severely limited by high viscosities, which hinders mass transfer across phase boundary layers. Dispersion of the IL onto a porous support has been suggested as a possible solution to this problem. In the present work, a vast variety of supported ionic liquid phase (SILP) materials have been tested in NO breakthrough experiments. Based on the obtained results, an attempt was made to understand the chemical and physical properties governing the SILP performance. Based on these investigations, characteristics of the optimal support were suggested. It was found that hollow-sphere silica (HS) had properties close to what was considered optimal, therefore it was decided to investigate this support material further. 

Synthesis of the support material and subsequently SILP formulations utilising the HS-support material were carried out in collaboration with Prof. Dai at Oak Ridge National Laboratory. The resulting HS-SILP performed significantly better than any other SILP formulation tested in NO breakthrough experiments. Based on this performance, it was suggested that the HS-support could be ideal for selective absorption of other gasses using SILP absorbers. Some SILP formulations were found to have significant oxidative capabilities, willingly oxidising NO to higher NOx species. It was found that the observed effect was due to alcohol residuals in the SILP material from the impregnation process, despite careful evaporation and drying. In order to investigate this effect further, the effect of several alcohols were screened and showed promising results. Therefore, an experimental setup was built to investigate if the oxidation would occur under continuous flow conditions, and to determine the steady state oxidation rates. Significant steady state conversions were found under continuous flow conditions, with a high turn over number for methanol. The reaction proceeded over all porous surfaces, but the use of a SILP material seemed to increase the rate of oxidation significantly.
Low Temperature DeNOx Technologies for Power and Waste Incineration Plants
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Macroalgae-based biorefineries

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Måling af bundmalingers friktionsmodstand
Bundmalinge anvendes på skibsbusnde for at undgå begroning, som øger friktionsmodstanden, og dermed brændstofforbruget, når skibet sejler. Malingerne kan enten være så glatte og elastiske, at begroning "vaskes af", når skibet sejler eller malingen kan afgive aktive stoffer, der afskrækker eller dræber begroningsorganismerne. Men hvilken maling giver mindst friktion set over hele skibets levetid?

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Mathematical modeling of pigment dispersion taking into account the full agglomerate particle size distribution
The purpose of this work is to develop a mathematical model that can quantify the dispersion of pigments, with a focus on the mechanical breakup of pigment agglomerates. The underlying physical mechanism was assumed to be surface erosion of spherical pigment agglomerates. The full agglomerate particle size distribution was simulated. Data from two previous experimental investigations were used for model validation. The first concerns two different yellow organic pigments dispersed in nitrocellulose/ethanol vehicles in a ball mill and the second a red organic pigment dispersed in a solvent-based acrylic vehicle in a three-roll mill. When the linear rate of agglomerate surface erosion was taken to be proportional to the external agglomerate surface area, simulations of the volume-moment mean diameter over time were
in good quantitative agreement with experimental data for all three pigments. The only adjustable parameter used was an apparent rate constant for the linear agglomerate erosion rate. Model simulations, at selected values of time, for the full agglomerate particle size distribution were in good qualitative agreement with the measured values. A quantitative match of the experimental particle size distributions could be obtained using time-dependent fragment distributions, but this resulted in a very slight improvement in the simulated transient mean diameter only. The model provides a mechanistic understanding of the agglomerate breakage process that can be used, e.g., in the development of novel dispersion principles and for analysis of dispersion failures. The general applicability of the model, beyond the three pigments considered, needs to be confirmed.

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Measurements of NOx precursor concentration profile above the bed at a full scale W-t-E plant and the effect of precursor speciation on the NOx formation

Satisfactory result from CFD modelling of NOx formation during combustion of waste in grate-fired waste-to-energy plants relies heavily on an accurate description of the temperature field in the free-board, this is a consequence of the high dependency of the temperature on the fuel NOx chemistry [1,2]. Modelling of the temperature field in the free-board in a CFD code relies on an accurate determination of the boundary conditions from the bed into the computational domain, e.g., species concentrations, gas temperature and gas velocity. Most CFD models of grate-fired waste-to-energy plants use a stand-alone model of the bed, describing the waste devolatilisation and the partial oxidation of volatiles, which have been coupled with the CFD model. The drying, devolatilisation and volatile oxidation in the bed is strongly coupled with the combustion of gaseous species in the free-board due to the radiation onto the bed as indicated in figure 1. The devolatilisation of the fuel and partial oxidation of the volatiles in the bed, generated during devolatilisation, has been coupled with the combustion of gaseous species in the freeboard and been applied with success in previous studies [3, 4].

Mechanistic Fermentation Models for Process Design, Monitoring, and Control

Mechanistic models require a significant investment of time and resources, but their application to multiple stages of fermentation process development and operation can make this investment highly valuable. This Opinion article discusses how an established fermentation model may be adapted for application to different stages of fermentation process development: planning, process design, monitoring, and control. Although a longer development time is required for such modeling methods in comparison to purely data-based model techniques, the wide range of applications makes them a highly valuable tool for fermentation research and development. In addition, in a research environment, where collaboration is important, developing mechanistic models provides a platform for knowledge sharing and consolidation of existing process understanding.
Mechanistic Model for Ash Deposit Formation in Biomass Suspension-Fired Boilers. Part 2: Model Verification by Use of Full Scale Tests

A model for deposit formation in suspension firing of biomass has been developed. The model describes deposit build-up by diffusion and subsequent condensation of vapors, thermoforesis of aerosols, convective diffusion of small particles, impaction of large particles and reaction. The model describes particle sticking or rebound by a combination of the description of (visco)elastic particles impacting a solid surface and particle capture by a viscous surface. The model is
used to predict deposit formation rates measured during tests conducted with probes in full-scale suspension-fired biomass boilers. The rates predicted by the model was reasonably able to follow the rates observed in the tests, although with some variation, primarily as overestimations of the deposit formation rates. It is considered that the captive properties of the deposit surface are overestimated. Further examination of some physical parameters related to the description of surface capture are suggested. Based on these examinations of the model ability to describe observed deposit formation rates, the proposed model can be regarded as a promising tool for description of deposit formation in full-scale biomass suspension fired boilers.

**General information**

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Mechanistic Model for Ash Deposit Formation in Biomass Suspension Firing. Part 1: Model Verification by Use of Entrained Flow Reactor Experiments

Two models for deposit formation in suspension firing of biomass have been developed. Both models describe deposit buildup by diffusion and subsequent condensation of vapors, thermophoresis of aerosols, convective diffusion of small particles, impaction of large particles, and reaction. The models differ in the description of the sticking probability of impacted particles: model #1 employs a reference viscosity in the description of the sticking probability, while model #2 combines impaction of viscoelastic particles on a solid surface with particle capture by a viscous surface. Both models were used to describe the deposit formation rates and deposit chemistry observed in a series of entrained flow reactor (EFR) experiments using straw and wood as fuels. It was found that model #1 was not able to describe the observed influence of temperature on the deposit buildup rates, predicting a much stronger influence of this parameter. Model #2 was able to provide a reasonable description of the influence of temperature on the deposit buildup rates observed in the EFR experiments. A parametric study was conducted to examine the influence of some physical parameters, including ash concentration, viscosity of ash and deposits, surface tension, Young's modulus, and porosity. On the basis of this model evaluation, where a wide range of temperatures (700–1000 °C) and fuels (straw and wood) were applied, model #2 can be regarded as a promising tool for the description of deposit formation from biomass ashes.
Metabolic Syndrome, Insulin Resistance and Cognitive Dysfunction: Does your metabolic profile affect your brain?
Dementia and type 2 diabetes are both characterized by long prodromal phases challenging the study of potential risk factors and their temporal relation. The progressive relation between metabolic syndrome, insulin resistance, and dementia has recently been questioned, wherefore the aim of this study was to assess the potential association between these precursors of type 2 diabetes and cognitive dysfunction. Using data from the Prospective Epidemiological Risk Factor study (n=2,103), a prospective study of elderly women in Denmark, we found that impaired fasting plasma glucose was associated with 44% (9%-91%) larger probability of developing cognitive dysfunction. In addition subjects above the HOMA-IR threshold (HOMA-IR > 2.6) had 47% (9%-99%) larger odds of cognitive dysfunction. The associations could indicate that a significant proportion of dementia cases in women is likely to be preventable by effective prevention and control of the insulin homeostasis.

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Methane Production and Carbon Capture by Hydrate Swapping

There are essentially two different approaches to producing methane from natural gas hydrate reservoirs, either bring the hydrate out of its thermodynamic stability region or expose the hydrate to a substance that will form a more stable hydrate structure, forcing an in situ swapping of the trapped gas molecules in the structural lattice. In this work, we quantitatively investigate the swapping behavior from injection of pure carbon dioxide and the (CO₂ + N₂) binary gas mixture through artificial hydrate-bearing sandstone samples by use of a core-flooding experimental apparatus. A total of 13 experimental runs were performed to examine the influence of operating conditions on methane production by CO₂/(CO₂ + N₂) injection in the temperature range of 274.15–277.15 K and 7.039–10.107 MPa pressure. Our results show that the use of the (CO₂ + N₂) binary gas mixture is advantageous compared to the use of pure carbon dioxide in swapping methane from its hydrate phase; the methane recovery efficiency in brine water systems is enhanced relative to pure water systems. The replenishment of a fresh (CO₂ + N₂) gas mixture into the vapor phase can be considered as an efficient extraction method because 46.32% of methane was displaced from its hydrate phase with the (CO₂ + N₂) binary gas mixture after 341.75 h of exposure to the (CO₂ + N₂) gas mixture. During the CH₄–(CO₂ + N₂) swapping process, gas chromatography analysis and calculations demonstrated that nitrogen molecules can take the place of some methane in small hydrate cages, as long as the equilibrium formation pressure of (CO₂ + N₂) binary gas hydrate is below that of methane hydrate, even though adding nitrogen to carbon dioxide reduces the thermodynamic driving force for the formation of a new hydrate. When other conditions are similar, the methane gas recovery efficiency increases with the
increase of the driving force for the swapping process.
Methodology for Analysing the NOx-NH3 Trade-off for the Heavy-duty Automotive SCR Catalyst

This paper presents a methodology where pareto fronts were used to analyse how changes in the control structure for the urea dosing to the automotive SCR catalyst can improve the trade-off between NOx slip and NH3 slip. A previously developed simulation model was used to simulate the European Transient Cycle (ETC) with P, PI, PD, and PID controllers, combined with Ammonia-NOx-Ratio (ANR) based feedforward to control the urea dosing. Results showed that PI with feedforward performed best. It was also shown that combining feedback with feedforward performed better than only using feedback or feedforward.

Methodology for Plantwide Design and Optimization of Wastewater Treatment Plants

Design of Wastewater Treatment Plants (WWTPs) is a complex engineering task which requires integration of knowledge and experience from environmental biotechnology, process engineering, process synthesis and design as well as mathematical programming. A methodology has been formulated and applied for the systematic analysis and development of plantwide design of WWTPs using mathematical optimization and statistical methods such as sensitivity and uncertainty analyses.
Micro scale reactor system development with integrated advanced sensor technology: A modular approach to the development of microfluidic screening platforms

Biotechnology is an increasingly relevant field, at a time when most industries strive for the development of greener processes by reducing and/or eliminating the environmental impact of industrial processes, often by limiting the use of certain compounds (e.g. harsh solvents, metal-based catalysts), but also by reducing the number of reaction steps and the quantity of generated waste. The use of biological systems, such as biocatalysts and cells, enables operation at milder conditions, creating new synthetic routes, improving regio- and stereoselectivity, and avoiding (de)protection steps requiring harsh solvents or compounds, among other advantages. However, due to the complexity of biological systems, the development of fermentation or biocatalyst based processes is not straightforward. Similar enzymes may act on similar substrates but operate at different temperatures. Combinations of enzymes in cascade systems may require the spatial separation of the involved enzymes due to incompatible side-products or inhibitions from the reaction components. Certain cells present a faster growth rate at high densities, or different production titres depending on the formation of aggregates or cell adherence. The broad range of biological molecules and cells available for bioprocesses thus require the optimization of specific substrates or operation conditions, which as illustrated, can vary widely between them. Furthermore, the discovery and tailoring of new biocatalysts or cells involves environmental sampling and the generation of new variants, resulting in thousands of biological systems whose industrial or clinical potential needs to be evaluated, often in a relatively short timeframe.

High-throughput analytical systems are the main tool applied to biocatalyst screening. They enable the parallel operation of different reactions and/or fermentations at different conditions (e.g. substrate concentrations, different substrates, enzymes, medium, oxygen availability, etc.). Thus, high-throughput systems allow to cover the possible variations and narrow the feasible operation conditions, substrates and biocatalysts or cells for application at industrial scale. The need for fast and comprehensive characterization of biocatalysts has also pushed the development of new screening platforms, based on microfluidics. Microfluidic systems involve the manipulation of small sample volumes (µL to nL) in miniaturized vessels and structures. Through miniaturization, mass and heat transfer becomes significantly faster, but surface and mass transfer limitations due to diffusion are also increased. Furthermore, microfluidics allows the use of different strategies for each of the unit operations involved in such optimization and screening studies, as well as new sensing and monitoring approaches.

Within microfluidics there are several approaches regarding the integration of the required unit operations, ranging from integration on a single chip to a fully modular approach, where different units correspond to a single chip but are interconnected through fluidic devices. The latter approach offers more flexibility at a lower cost in terms of the achievable studies with the same unit operations, since these can be placed in a different order depending on the purpose or sample being characterized.

The main goal of this dissertation was to develop a biocatalyst screening platform based on modular microfluidics. With this purpose in mind, three microfluidic modules are presented that can be integrated and used in such modular platform: a microreactor module with integrated oxygen sensors, a microfluidic dilution and quantification module compatible with electrochemical sensors and a module for continuous thermal inactivation of enzymes. The last two modules were developed specifically for applications in online screening. The focus during development was on achieving user-friendly and simple to use platforms that were furthermore easy to connect with other existing platforms and compatible with a wide range of biocatalytic reactions.

The microreactor module enables the continuous monitoring of oxygen levels and was characterized with a biocatalytic oxidation reaction in order to highlight the operational limitations of the system in terms of oxygen depletion at certain enzyme and substrate concentrations. Strategies for in situ oxygen generation involving addition of catalase and hydrogen...
peroxide were applied as solutions to overcoming the identified oxygen depletion limitations. Furthermore, the reactions carried out in the microfluidic system were modelled using computational fluid dynamics, with a good fit between the experimental and simulated data, and the results provided extra insight into the reaction dynamics. The same microreactor was applied to the screening of whole cell variants of a dioxygenase capable of converting alkene substrates. It was used as a complement to the screening of genetically modified biocatalysts using end-point product quantification. The oxygen consumption rate of each variant in the presence of a standard substrate was used as the screening parameter to select the variant with the faster oxidation reaction rate as the best variant for a possible industrial application.

The second module was developed for integration of different types of sensors to achieve online quantification. The module presents a standardized fitting enabling the connection to either other microfluidic platforms or laboratory scale equipment. Screen-printed electrochemical sensors were integrated through pockets that allowed their easy replacement and thus the re-use of the microfluidics’ platform. Also, the developed platform included a mixing/dilution channel enclosed by a two-sensor system, which allowed expanding the sensors’ detection range by controlling the sample dilution at which the measurements were performed. The dilution unit was optimized with computational fluid dynamic methods that enabled testing several geometries before fabrication, thus accelerating the platform development.

The third microfluidic module was developed to allow unspecific inactivation of biocatalysts (especially enzymes), and thus precisely control the reaction (residence) time at the point of product quantification in the second module. Such control is important when different modules – reactors and/or sensing units – are used and frequently changed. It can furthermore help to regulate the state of the biocatalyst, since it is depending on the temperature and exposure time. In this way, reversible or irreversible denaturation of the enzymes can be achieved.

The different modules presented in the dissertation are useful additions to a modular microfluidic toolbox for biocatalyst screening. They provide online monitoring of biocatalytic reactions or biotransformations, quantification of reaction products and controlled reaction end-points due to the potential to achieve precise temperature control. Furthermore, the developed computational fluid dynamic models allow for a better understanding of the reaction performed in the microsystem. The model can be further improved to achieve online data acquisition of reaction kinetics by coupling with a mechanistic model. In the case of the developed mixing/dilution channel, the developed model enabled a fast optimization of the unit operation, thereby decreasing the cost and time spent on such endeavour.

The potential of modular microsystems in biotechnological applications was the main driver for the work performed and presented in this dissertation. The objective of this dissertation was to provide, beside three interesting microfluidic systems, a better understanding of the potential that microfluidics, especially in a modular approach and tightly connected to mathematical modelling, can offer to biotechnology and society.

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Mixing and mass transfer in a pilot scale U-loop bioreactor
A system capable of handling a large volumetric gas fraction while providing a high gas to liquid mass transfer is a necessity if the metanotrophic bacterium Methylococcus capsulatus is to be used in single cell protein (SCP) production. In this study mixing time and mass transfer coefficients were determined in a 0.15 m3 forced flow U-loop fermenter of a novel construction. The effect on the impeller drawn power when a gas was introduced into the system was also studied. Mixing time decreased and mass transfer increased with increasing volumetric liquid flow rate and specific power input. This happened also for a large volume fraction of the gas, which was shown to have only minor effect on the power drawn from the pump impeller. Very large mass transfer coefficients, considerably higher than those obtainable in an STR and previous tubular loop reactors, could be achieved in the U-loop fermenter equipped with static mixers at modest volumetric liquid and gas flow rates. This article is protected by copyright. All rights reserved
Model-based design and analysis of glucose isomerization process operation

The application of model-based methods for design and analysis of operational improvements of an industrial glucose isomerization (GI) process is highlighted. First, a multi-scale mathematical model representing important phenomena encountered in the reaction system of a glucose isomerization reactor is developed. Next, model analysis, model identification and model validation based on available reactor operational data are performed. The reactor model is found to describe accurately important phenomena, such as, reaction kinetics, enzyme decay and internal diffusion of the substrate in the enzymatic pellet as a function of the temperature, thereby confirming that the model is ready for use in design-analysis studies. Operation of the GI process is then analyzed in a single reactor and based on this, the reactor model is used as a building block to represent the operation of a GI reactor plant consisting of 10–20 reactors in parallel. The design of the GI plant operation is evaluated through the analysis of simulated results of different operational scenarios.
Model-based identification of chemicals transformation pathways combined with reaction kinetics models– the case of heroin biomarkers in wastewater

General information
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Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Environmental Chemistry
Authors: Ramin, P. (Intern), Valverde Pérez, B. (Intern), Polesel, F. (Intern), Gernaey, K. (Intern), Plósz, B. G. (Intern)
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Model-based Optimization of Pectin Extraction Process
Commercial pectin produced through an extraction using acid is used as a gelling, thickening, emulsifying or stabilizing agent in many applications due to its gelling ability. Quality of the gel formed by pectin depends on physical and chemical characteristics of extracted pectin, such as degree of esterification (DE) and intrinsic viscosity (IV). However, since there is a trade-off between the pectin yield and quality, it becomes a challenge to decide the extraction condition using heuristic approaches. In this study, we propose a strategy for an operation optimization of the pectin extraction process using the dynamic model developed based on the first principles. In the optimization problem, the desired characteristics of pectin are considered as inequality constraints of end states. The extraction condition, i.e. temperature, pH and extraction time, are optimized to maximize a final pectin concentration satisfying given requirements according to product specific applications.
Model-based plant-wide optimization of large-scale lignocellulosic bioethanol plants.

Second generation biorefineries transform lignocellulosic biomass into chemicals with higher added value following a conversion mechanism that consists of: pretreatment, enzymatic hydrolysis, fermentation and purification. The objective of this study is to identify the optimal operational point with respect to maximum economic profit of a large scale biorefinery plant using a systematic model-based plantwide optimization methodology. The following key process parameters are identified as decision variables: pretreatment temperature, enzyme dosage in enzymatic hydrolysis, and yeast loading per batch in fermentation. The plant is treated in an integrated manner taking into account the interactions and trade-offs between the conversion steps. A sensitivity and uncertainty analysis follows at the optimal solution considering both model and feed parameters. It is found that the optimal point is more sensitive to feedstock composition than to model parameters, and that the optimization supervisory layer as part of a plantwide automation system has the following benefits: (1) increases the economical profit, (2) flattens the objective function allowing a wider range of operation without negative impact on profit, and (3) reduces considerably the uncertainty on profit.

General information
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Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, DONG Energy Thermal Power A/S
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Web of Science (2015): Indexed yes
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Modeling Deactivation of Catalysts for Selective Catalytic Reduction of NOx by KCl Aerosols

A detailed model for the deactivation of a V2O5-WO3/TiO2-based SCR monolith catalyst by potassium poisoning has been developed and validated. The model accounts for deposition of KCl aerosol particles present in the flue gas on the external catalyst surface, the reaction of the deposited particles with the catalyst at the surface of the monolith wall, the transport and accumulation of potassium, bound to Brønsted acid sites, throughout the catalyst wall, and the resulting loss in SCR activity. Using an experimentally measured KCl aerosol size distribution as input, the model can replicate the observed deactivation rate of a 3 wt % V2O5-7 wt % WO3/TiO2 monolith catalyst, exposed to a KCl aerosol at 350 °C for about 1000 h, as well as the resulting potassium-to-vanadium molar ratios in the catalyst wall. Simulations show that the particle deposition rate, as well as the deactivation rate, decreases if the particle size of the incoming aerosol is increased. The model provides, for the first time, a mechanistic framework for understanding and modeling SCR catalyst deactivation by KCl that may be applicable also for deactivation by other salts and at different operating conditions.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS
Authors: Olsen, B. K. (Intern); Castellino, F. (Ekstern); Jensen, A. D. (Intern)
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
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ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
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Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
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Web of Science (2005): Indexed yes
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Web of Science (2004): Indexed yes
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Modeling of Asphaltene Precipitation from Crude Oil with the Cubic Plus Association Equation of State

In this study, different modeling approaches using the Cubic Plus Association (CPA) equation of state (EoS) are developed to calculate the asphaltene precipitation onset condition and asphaltene yield from degassed crude oil during the addition of n-paraffin. A single model parameter is fitted to calculate the asphaltene onset condition during the addition of different n-paraffin precipitants (n-pentane to n-hexadecane). Three parameters per precipitant are fitted to calculate the asphaltene yield during the addition of the precipitant. The results obtained from the model are compared with the experimental data for eight different crude oils. Results were also obtained for seven crudes using the Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) EoS based approach described in the literature. The CPA EoS based approaches treat the asphaltene fraction as an associating component whereas the PC-SAFT EoS based approach does not. A comparison between the approaches shows that the CPA EoS based approaches, developed in this work, give more reliable results. The predictions from the PC-SAFT EoS based approach result in behavior that is unphysical: the mole fraction of n-paraffin (at the precipitation onset) and the asphaltene yield do not decrease with the carbon number of n-paraffin. Furthermore, it is shown that the approach, developed in this work, can predict the onset conditions of asphaltene precipitation resulting from a blend of two or more crudes.

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
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Modeling of Gas Diffusion in Ni/YSZ Electrodes in CO₂ and Co-electrolysis

Carbon formation may occur during CO₂ and CO₂/H₂O electrolysis using solid oxide electrolyzer cells due to the Boudouard reaction (2CO → CO₂ + C(δ)). Formed carbon may disintegrate the cell structure and it is therefore of importance to be able to predict when carbon is formed, and take actions to prevent its formation. For prediction of carbon formation, the gas composition in the electrode must be known. In this work, the diffusion of gases in the electrode has been modeled with the dusty gas model in 1 and 2 dimensions, and the effect of tortuosity, porosity, temperature, electrode thickness, pore diameter, current density, pitch and rib width has been investigated. It is shown that diffusion limitations on reactant/product transport may lead to carbon formation. The parameters describing the microstructure and the dimensions of the cathode channels and interconnect ribs are found to have a large effect on the carbon formation propensity. Given a set of parameters, a simple correlation between the CO mole fraction in the channel and under the interconnect rib, and current density during CO₂-electrolysis can be derived. This correlation makes it possible to efficiently integrate the calculation of carbon formation risk in existing electrolyzer cell models.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS
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Modeling of Shale Gas Adsorption and its Influence on Phase Equilibrium

Natural gas and oil produced from shale accounts for a significant portion in the global production. Due to the large surface area and high organic content in shale formations, adsorption plays a major role in the storage of the hydrocarbons within the rock and their phase equilibrium. This study provides a comparison of several engineering models for gas adsorption in shale based on the recent literature data for pure and binary gases. For pure components, Langmuir, the modified Toth-Langmuir, and the Multicomponent Potential Theory of Adsorption using Dubinin-Radushkevich potential (MPTA-DRA) were compared. The three models show similar deviations lower than 10%. For binary gases, Multicomponent Langmuir (ML), Ideal Adsorbed Solution Theory (IAST) and MPTA were evaluated, where MPTA shows the lowest deviation with 17.9%. Additionally, we presented an analysis of the phase envelope shift under the influence of the capillary pressure and the adsorption film. ML and IAST were used to calculate the adsorption amount whereas MPTA was used to generate artificial adsorption data over large temperature range and for other homologous hydrocarbons to estimate the ML and IAST parameters. The adsorption film thickness was considered in the calculation of the effective capillary radius and the corresponding capillary pressure. The combined effects modify the saturation pressure in the whole temperature range except at the critical point. The biggest impact was found on the bubble point branch away from the critical point where the
interfacial tension of the system is more pronounced.

**General information**

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**Organisations:** Department of Chemistry, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering  
**Authors:** Sandoval Lemus, D. R. (Intern), Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)  
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- Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139  
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- Scopus rating (2009): SJR 1.002 SNIP 1.164  
- Web of Science (2009): Indexed yes  
- BFI (2008): BFI-level 2  
- Scopus rating (2008): SJR 1.142 SNIP 1.267  
- Web of Science (2008): Indexed yes  
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- Web of Science (2007): Indexed yes  
- Scopus rating (2006): SJR 1.035 SNIP 1.204  
- Web of Science (2006): Indexed yes  
- Scopus rating (2005): SJR 0.993 SNIP 1.241  
- Web of Science (2005): Indexed yes  
- Scopus rating (2004): SJR 1.046 SNIP 1.452
Modeling Study of High Pressure and High Temperature Reservoir Fluids

With dwindling easily accessible oil and gas resources, more and more exploration and production activities in the oil industry are driven to technically challenging environments such as unconventional resources and deeper formations. The temperature and pressure can become extremely high, e.g., up to 250 °C and 2400 bar, in the deep petroleum reservoirs. Furthermore, most of these deep reservoirs are found offshore, including the North Sea and the Gulf of Mexico, making the development even more risky. On the other hand, development of these high pressure high temperature (HPHT) fields can be highly rewarding if successfully produced. This PhD project is part of the NexOil (New Extreme Oil and Gas in the Danish North Sea) project which is intended to reduce the uncertainties in HPHT field development. The main focus of this PhD is on accurate description of the reservoir fluid behavior under HPHT conditions to minimize the production risks from these types of reservoirs. In particular, the study has thoroughly evaluated several non-cubic Equations of State (EoSs) which are considered promising for HPHT fluid modeling, showing their advantages and short comings based on an extensive comparison with experimental data. In the course of the evaluation, we have developed new petroleum fluid characterization procedures, built large databases for well-defined mixtures and reservoir fluids, and improved the evaluation software and made it more suitable for efficient and large scale comparison. We have made a comprehensive comparison between cubic and non-cubic EoSs to evaluate whether advanced EoS in non-cubic forms, including both the SAFT-type EoS with strong theoretical basis (e.g. the PC-SAFT EoS) and the empirical BWR-type EoS (e.g. the Soave-BWR EoS), can be advantageous for describing the physical properties and phase equilibrium of reservoir fluids over a wide temperature and pressure range. In addition, we have also compared these models in calculation of heat capacities and Joule-Thomson coefficients for pure components and multicomponent mixtures. Joule-Thomson coefficients are of special interest to the oil industry because of the so called reverse Joule-Thomson effect commonly observed in HPHT fields, where a decrease in pressure results in an increase in temperature, which is just the opposite to the effect at low pressure. In the comparative studies between cubic and non-cubic EoSs, we also included GERG-2008 which is a wide-range EoS developed for 21 components of natural gases and their binary mixtures and is regarded as the most accurate EoS model for natural gas mixtures. It was found that the non-cubic models are much better than the cubics in density, compressibility, heat capacity and Joule-Thomson coefficient calculation of the well defined light and heavy components in reservoir fluids over a wide temperature and pressure range, GERG-2008 being the best with the lowest deviation among all EoS models. GERG-2008 however gives very large deviations for bubble point pressure calculation of some heavy and asymmetric binary systems such as n-butane + n-nonane system. This suggests that this EoS and its binary interaction parameters could still be improved for some of the binary pairs. Soave-BWR gives the closest prediction of the thermal properties to that of GERG-2008 among other EoSs tested in this study. The binary VLE calculation showed that PC-SAFT and Soave-BWR are similar to SRK and PR in correlating the important binary pairs in reservoir fluids. Although Soave-BWR and PC-SAFT give smaller average kij values than SRK and PR, they are more sensitive to the change in kij. Phase envelope prediction of synthetic gases showed that all the EoS models were similar for not too asymmetric synthetic gases, with or without the optimal kij values for SRK, PR, PC-SAFT and Soave-BWR. For highly asymmetric synthetic mixtures, Soave-BWR and GERG-2008 tend to predict phase envelopes different from other models where as none of the tested models give satisfactory predictions. For heat capacity and Joule-Thomson coefficients, GERG-2008 and Soave-BWR give the closest predictions. All the evaluated EoS models tend to predict a nearly constant Joule-Thomson coefficient at high pressures. For typical reservoir temperatures, the constant is around -0.5 K/MPa. For non-cubic models like PC-SAFT the characterization method is less mature than the cubic models. A reservoir fluid characterization method for PC-SAFT has been proposed by combining Pedersen’s method with a newly developed set of correlations for the PC-SAFT model parameters m, m/k and mσ3. In addition, we further improved the characterization method for PC-SAFT by adjusting the correlations with a large PVT database. We have further improved the correlations and more importantly, we have established a general approach to characterizing reservoir fluids for any EoS. The approach consists in developing correlations of model parameters first with a database for well-defined components and then adjusting the correlations with a large PVT database. The adjustment is made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and Stock Tank Oil density, while keeping the n-alkane limit of the correlations unchanged. Apart from applying this general approach to PC-SAFT, we have also shown that the approach can be applied to classical cubic models like SRK and PR. In addition, we discussed how to develop a PNA based characterization for PC-SAFT and also utilize a large PVT database to further improve the
characterization. With the developed characterization methods, we have made a comparison in PVT calculation involving 17EoS-characterization combinations and 260 reservoir fluids. PC-SAFT with the new general characterization method is shown to give the lowest AAD% and maximum deviation in calculation of saturation pressure, density and STO density, among all the tested characterization methods for PC-SAFT. Application of the new characterization method to SRK and PR improved the saturation pressure calculation in comparison to the original characterization method for SRK and PR. Using volume translation together with the new characterization approach for SRK and PR gives comparable results for density and STO density to that of original characterization for SRK and PR with volume translation. For the PVT database used in this study, cubic EoSs seem to have better performance than PC-SAFT in calculation of saturation pressure; PC-SAFT and cubics with volume translation show comparable results in calculation of density and STO density. As a preliminary attempt to integrate more analytical information in characterization, we discussed how to modify the existing algorithms to utilize data from both simulated distillation and true boiling point distillation, and in particular, the component distribution information from the simulated distillation. Some analyses have been made on the impact of including more detailed analytical information. Finally, to improve Soave-BWR for mixture calculation, we have tried to develop several new sets of mixing rules for this EoS. The new mixing rules were developed based on some theoretical considerations as well as the previous mixing rules for non-cubic EoS models. In addition, it was tried to create some hybrid mixing rules by combining a new set of mixing rules and the original mixing rules for Soave-BWR. It was shown that some problems with the original Soave-BWR mixing rules can be fixed by the new mixing rules although the overall performance is not significantly improved. Development of mixing rules for non-cubic EoS models is still a semi-empirical process, requiring extensive testing to evaluating their performance. We have developed the code in a structured manner so that the new mixing rules can be quickly tested. It can facilitate further extensive screening of new mixing rules for Soave-BWR or even other non-cubic EoS models.
Fast pyrolysis, Heating rate, Kinetics, Metaplast, Potassium

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Modelling and Operation of Diesel Engine Exhaust Gas Cleaning Systems

Diesel engine exhaust gases contain several harmful substances. The main pollutants are carbon monoxide (CO), hydrocarbons (HC), particulate matter (PM), and nitrous gases such as nitrogen oxide (NO) and nitrogen dioxide (NO₂) (together NOx). Reducing the emission of these pollutants is of great importance due to their effect on urban air quality, and because of new legislation. In modern heavy-duty applications, the exhaust gases are typically treated with four different catalysts: a Diesel Oxidation Catalyst (DOC) which oxidises HC and CO into H₂O and CO₂, and NO into NO₂, a Diesel Particulate Filter (DPF) which filters PM, a Selective Catalytic Reduction (SCR) catalyst which removes NO and NO₂ through reaction with NH₃, and an Ammonia Slip Catalyst (ASC) which removes excess ammonia (NH₃) before the gases are released to the atmosphere.

SCR is a widely used technology to reduce NOx to N₂. Challenges with this technology include dosing the appropriate amount of urea to reach sufficient NOx conversion, while at the same time keeping NH₃-slip from the exhaust system below the legislation. This requires efficient control algorithms.

The focus of this thesis is modelling and control of the SCR catalyst. A single channel model for a heavy-duty SCR catalyst was derived based on first principles. The model considered heat and mass transfer between the channel gas phase and the wash coat phase. Four simplified models were derived, with simplifications related to mass and heat transfer. The model parameters were estimated using bench-scale monolith isothermal data. Validation was done by simulating the out-put from a full-scale SCR monolith that was treating real engine gases from the European Transient Cycle (ETC). Results showed that the models were successfully calibrated, and that some of the models could predict the ETC output satisfactorily. The models' predictive capabilities were investigated in relation to the simplifications, and results showed that the simplifications related to mass transfer resulted in the smallest information loss.

A methodology to analyse the NOx-NH₃ trade-off for different urea dosing controllers was developed, and applied to P, PI, PD, and PID controllers, both with and without Ammonia-NOx-Ratio (ANR) based feedforward. Simulation results showed that the PI controller with feedforward had the best NOx-NH₃ trade-off, and that feedforward coupled with feedback outperformed the other control structures. The results were experimentally verified by implementing the tested controllers on a full-scale engine setup, and the results showed that coupling feedback with ANR based feedforward was yielding better performance. The PD controller showed good performance in the experimental validation.

Finally, a methodology for creating a modular simulation tool was developed. The methodology goes through the steps that are required to integrate individual models so that they can be used for the tool. The methodology is demonstrated by applying it to four models from literature, and simulating the system.

Decision support systems are a key focus in research on developing control rooms to aid operators in making reliable decisions, and reducing incidents caused by human errors. For this purpose, models of complex systems can be developed to diagnose causes or consequences for specific alarms. Models applied in safety systems of complex and safety critical systems, require rigorous and reliable model building and testing. Multilevel Flow Modeling is a qualitative method for diagnosing faults, and has previously only been validated by subjective and qualitative means. This work aims to synthesize a procedure to measure model performance, according to diagnostic requirements, to ensure reliability during operation. A simple procedure is proposed for validating and evaluating Multilevel Flow Modeling models. For this
purpose expert statements, a dynamic process simulation in K-spice, and pilot plant experiments are used for validation of two simple Multilevel Flow Modeling models of a deoiling hydrocyclone, used for water and oil separation.

**General information**

State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Aalborg University
Authors: Nielsen, E. K. (Intern), Bram, M. V. (Forskerdatabase), Frutiger, J. (Intern), Sin, G. (Intern), Lind, M. (Intern)
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**Modelling an industrial anaerobic granular reactor using a multi-scale approach**

The objective of this paper is to show the results of an industrial project dealing with modelling of anaerobic digesters. A multi-scale mathematical approach is developed to describe reactor hydrodynamics, granule growth/distribution and microbial competition/inhibition for substrate/space within the biofilm. The main biochemical and physico-chemical processes in the model are based on the Anaerobic Digestion Model No 1 (ADM1) extended with the fate of phosphorus (P), sulfur (S) and ethanol (Et-OH). Wastewater dynamic conditions are reproduced and data frequency increased using the Benchmark Simulation Model No 2 (BSM2) influent generator. All models are tested using two plant data sets corresponding to different operational periods (#D1, #D2). Simulation results reveal that the proposed approach can satisfactorily describe the transformation of organics, nutrients and minerals, the production of methane, carbon dioxide and sulfide and the potential formation of precipitates within the bulk (average deviation between computer simulations and measurements for both #D1, #D2 is around 10%). Model predictions suggest a stratified structure within the granule which is the result of: 1) applied loading rates, 2) mass transfer limitations and 3) specific (bacterial) affinity for substrate. Hence, inerts (Xi) and methanogens (Xac) are situated in the inner zone, and this fraction lowers as the radius increases favouring the presence of acidogens (Xac, Xaa, Xfa) and acetogens (Xc4, Xpro). Additional simulations show the effects on the overall process performance when operational (pH) and loading (S:COD) conditions are modified. Lastly, the effect of intra-granular precipitation on the overall organic/inorganic distribution is assessed at: 1) different times; and, 2) reactor heights. Finally, the possibilities and opportunities offered by the proposed approach for conducting engineering optimization projects are discussed.

**General information**

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Modelling biotransformation of drug biomarkers by sewer biofilms

General information
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Modelling of an adiabatic trickle-bed reactor with phase change
This paper describes a modelling approach of the behavior of trickle-bed reactors used for catalytic hydrotreating of oil fractions. A dynamic plug-flow heterogeneous one-dimensional adiabatic model was used to describe the main reactions present in the hydrotreating process: hydrodesulfurization, hydrodenitrogenation, and hydrodearomatization. The model was solved using a finite differences scheme and was coupled with a flash calculation in ProII and thus, obtaining a simulation framework that can be generally used for such reactors.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, CHEC Research Centre, Haldor Topsoe AS
Authors: Ramirez Castelan, C. E. (Intern), Hidalgo-Vivas, A. (Ekstern), Brix, J. (Ekstern), Jensen, A. D. (Intern), Huusom, J. K. (Intern)
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Modelling of temporal and spatial evolution of sulphur oxides and sulphuric acid under large, two-stroke marine engine-like conditions using integrated CFD-chemical kinetics
In this work, three-dimensional computational fluid dynamics (CFD) studies of sulphur oxides (SO\textsubscript{x}) and sulphuric acid (H\textsubscript{2}SO\textsubscript{4}) formation processes in a large, low speed two-stroke marine diesel engine are carried out. The current numerical study aims to investigate the conversion of sulphuric dioxide (SO\textsubscript{2}) to sulphuric trioxide (SO\textsubscript{3}) and the possibility of H\textsubscript{2}SO\textsubscript{4} condensation which are the prerequisites to better understand the corrosion-induced wear phenomenon. This is achieved with the aid of the implementation of a multicomponent surrogate model, which comprises a skeletal n-heptane mechanism and a reduced sulphur subset mechanism. In the present work, performance of the coupled CFD-chemical kinetic model is evaluated using both qualitative and quantitative methods. The modelling results show that the temporal and spatial evolutions of SO\textsubscript{x} predicted by the skeletal model are similar to those by the base mechanism. Predictions of the variations of SO\textsubscript{x} and the associated SO\textsubscript{2} to SO\textsubscript{3} conversion in response to the change of fuel sulphur content, swirl velocity, start of injection, scavenge pressure and humidity qualitatively agree with numerical and experimental results from the literature. The model is further evaluated using the measured SO\textsubscript{2} to SO\textsubscript{3} conversion levels in a low load, low scavenge pressure case and a low load, high scavenge pressure case. The absolute values of simulated and measured conversion levels are close, although the former appear to be higher. The current results show that the flame impingements at the cylinder liner near top dead centre. The gas is cooled rapidly by the wall temperature and H\textsubscript{2}SO\textsubscript{4} is produced in the region where the local temperature is less than 600 K. Based on the fluegas correlation, the acid dew point temperature is higher than the wall temperature, suggesting that acid condensation may begin early at the top part of the cylinder liner.
The predicted distribution correspondswell with the distribution of corroded parts observed in service engines. The model is expected to serve asan important tool to simulate the rates of SO$_2$ absorption into lubricating oil film and H$_2$SO$_4$ condensationin this combustion system.

**General information**

State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CHEC Research Centre, MAN Diesel & Turbo SE
Authors: Pang, K. M. (Intern), Karvounis, N. (Intern), Walther, J. H. (Intern), Schramm, J. (Intern), Glarborg, P. (Intern), Mayer, S. (Ekstern)
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 2.854 SNIP 3.108 CiteScore 5.69
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Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 2.473 SNIP 2.84 CiteScore 5.5
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.516 SNIP 2.25
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.003 SNIP 1.781
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.974 SNIP 1.215
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.179 SNIP 1.709
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.979 SNIP 1.293
Scopus rating (2005): SJR 1.043 SNIP 0.996
Modification of polymer surfaces to enhance enzyme activity and stability

Enzyme immobilization is an important concept for the development of improved biocatalytic processes, primarily through facilitated separation procedures. However, enzyme immobilization usually comes at a price of reduced biocatalytic activity. For this reason, different immobilization methods have already been developed, combining the same goal to improve enzyme activity, stability and selectivity. Polymer materials have shown, due to their easy processibility and versatile properties, high potential as enzyme support. However, in order to achieve improved enzyme performance, the combination of different factors, such as the nature of the enzyme, the properties of the support, the type of immobilization and the interaction between enzyme and support, has to be taken into consideration. In this thesis, these factors are pursued and addressed by exploiting various types of polymers with focus on their tailored surface modification in order to obtain improved enzyme-support systems.

Firstly, an off-stoichiometric thiol-ene (OSTE) thermosetting material was used for the development of a screening platform allowing the investigation of micro-environmental effects and their impact on the activity of immobilized enzymes. Micro-environmental changes were generated through the introduction of tailored surface functionalities via thiol-ene chemistry (TEC) and surface chain transfer free radical polymerization (SCT-FRP), which demonstrated a significant influence on the activity of immobilized horseradish peroxidase (HRP). Thereby, this versatile screening substantiated the identification of suitable support surfaces for the immobilization of enzymes.

Secondly, in order to facilitate the application of previously identified enzyme-support combinations, OSTE particles as enzyme carriers were prepared. Here, a novel fabrication process via suspension polymerization in glycerol was applied resulting in microparticles with high control over particle size, which were further surface functionalized through TEC and SCT-FRP. In this case, epoxide functional particles were applied for the covalent immobilization of HRP and thus, demonstrated their potential as enzyme carrier in a continuous biocatalytically active plug-flow reactor. Thirdly, OSTE particles with different surface functionalities were further used for the immobilization of β-glucosidase. The aim of this study was primarily to improve enzymatic selectivity through tailored changes of the micro-environment between enzyme and surface, which was achieved by introducing different surface chemistries onto the particles. The resulting selectivity between trans-glycosylation and hydrolysis of p-nitrophenyl glucopyranoside (pNPG) catalyzed by immobilized β-glucosidase was significantly improved and showed a direct correlation to the surface chemistry. Furthermore, enzyme effectiveness is another important factor for the development of biocatalytic processes, which was addressed by immobilizing HRP in microfluidic devices based on OSTE+ materials. In this approach, area selective surface functionalization allowed the immobilization of HRP in various surface patterns and consequently, the effect of spatial enzyme distribution was determined towards the overall reactor performance. Two checkerboard patterns were identified to exploit enzymes more efficiently compared to an even distribution on the surface.

Finally, improvements in enzyme stability was the focus of applying tailored surface functionalization and polymer grafting of polysulfone (PSf) membranes and their subsequent application as biocatalytic membrane reactors (BMRs). Immobilization of alcohol dehydrogenase (ADH) onto poly(1-vinyl imidazole) (pVIm) grafted membranes demonstrated increased biocatalytic activity and stability compared to pristine membranes and thus, showed improved enzyme performance through tailored micro-environment by polymer grafting.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for BioProcess Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre
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Number of pages: 155
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Monte Carlo Based Framework to Support HAZOP Study

This study combines Monte Carlo based process simulation features with classical hazard identification techniques for consequences of deviations from normal operating conditions investigation and process safety examination. A Monte Carlo based method has been used to sample and evaluate different deviations in process parameters simultaneously, thereby bringing an improvement to the Hazard and Operability study (HAZOP), which normally considers only one at a time deviation in process parameters. Furthermore, Monte Carlo filtering was then used to identify operability and hazard issues including inefficient, uneconomical and unsafe conditions. Appropriate process modifications to mitigate deviations from normal operation ensuring process safety are also provided.

Multi-scale Modeling Approach for Design and Optimization of Oleochemical Processes

The primary goal of this work is to present a systematic methodology and software framework for a multi-level approach ranging from process synthesis and modeling through property prediction, to sensitivity analysis, property parameter tuning and optimization. This framework is applied to the following selected oleochemical processes: vegetable oil splitting, fatty acid fractionation and glycerol purification. The framework includes the prediction of physical and thermodynamic properties and the uncertainties of the estimated values coupled with the process model represented by mass and energy balances. The effects of these uncertainties are assessed with sensitivity analysis. Standardized regression coefficients (SRC) are evaluated and Sobol analysis is performed to study the counter-current spray splitting column and rank each model parameter. The information obtained is used for the tuning of property models, optimization of process flowsheets and analysis of the overall process by multi-criteria sustainability and economics analysis.
Municipal Solid Waste Management in a Low Income Economy Through Biogas and Bioethanol Production

The biodegradable fraction of municipal solid wastes generated from households in Ghana has favourable characteristics worth considering for bioenergy production. The suitability of this biodegradable portion for biogas and bioethanol production was assessed in this study. The assessment was performed on both untreated and hydrothermally treated unsorted and sorted fractions of the waste using standard methods for biomass conversion to bioenergy. Compositional analysis of the waste indicated that unsorted biodegradable municipal solid wastes (BMSW) consisted of 38.7 % dry matter (DM) glucan, 8.3 % DM hemicellulose, 10.1 % DM lignin and 7.6 % DM ash. The sorted fractions with the highest glucan but least lignin and hemicellulose were the pool of cassava, yam and plantain peeling wastes (CYPPW) with 84 % DM glucan much of which was starch, 5.6 % DM lignin and 0.5 % DM hemicellulose. The highest ethanol yield of 0.29 l/kg DM was measured from this same CYPPW while fruit wastes (FW) had the highest biomethane potential of 408 ml CH4/g VS. The BMSW had ethanol yield of 0.17 l/kg DM and biogas 369 ml CH4/g VS. The hydrothermally pretreated wastes had marginal increases in glucose and ethanol yield except the treated yard waste which significantly increased by 54 % in glucose over the untreated waste. The most promising waste fractions were FW, CYPPW and mixed paper wastes. Careful selection of these fractions in feedstock for biofuel production would reduce generation of the waste, improve the quality and effectively lead to higher yield of biofuel over the unsorted form.

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Scopus rating (2015): SJR 0.396 SNIP 0.515 CiteScore 1.08
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 0.455 SNIP 1.004 CiteScore 1.25
Scopus rating (2013): SJR 0.731 SNIP 1.074 CiteScore 2.01
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.691 SNIP 1.27 CiteScore 1.86
ISI indexed (2012): ISI indexed no
New degradation compounds from lignocellulosic biomass pretreatment: routes for formation of potent oligophenolic enzyme inhibitors

In this study 26 new oligophenol cellulase inhibitors were discovered from wheat straw pretreatment liquors. By consideration of the reaction mechanisms for their formation it is proposed that these oligophenols are formed during hydrothermal biomass pretreatment by pentose self-condensation reactions involving aldol condensations, 1,4 additions to α,β unsaturated carbonyl compounds, 3-keto acid decarboxylations and oxidations. Furthermore, pentose reactions with phenolic lignin components are suggested. The identification of the central role of xylose in the reaction routes for oligophenolic inhibitor formation led to the solution to protect the reactive anomic center in xylose. It is shown that protection of the anomic center in in situ generated xylose with ethylene glycol monobutyl ether, during pretreatment of wheat straw, reduces the level of oligophenols by 73%. The results pave the way for implementation of new types of reactions that hinder inhibitor formation in lignocellulosic biomass processing.

General information
State: Published
New insights in the low-temperature oxidation of acetylene

This work presents new experimental data of C$_2$H$_2$ low-temperature oxidation for equivalence ratios $\Phi$=0.5–3.0 in a newly designed jet-stirred reactor over a temperature range of 600–1100K at atmospheric pressure with residence time corresponding from 1.94 to 1.06s. Mole fraction profiles of 17 intermediates including aromatic compounds such as toluene, styrene and ethylbenzene were quantified. A detailed kinetic mechanism involving 295 species and 1830 reactions was established to predict the oxidation of C$_2$H$_2$ and formation of PAH. In developing the mechanism, particular attention was paid to reactions of the vinyl radical and to steps involved in the sequence C$_2$H$_2$→iC$_4$H$_5$→fulvene→C$_6$H$_5$CH$_2$→C$_6$H$_6$. In general, the peak concentrations of intermediates gradually increase and peak locations tend to shift toward high temperatures with $\Phi$ increasing. Flux analysis indicates that the addition of H and the reaction with O are the two major channels governing C$_2$H$_2$ consumption. At temperatures below 1000K, benzene is mainly formed through the C$_2$+C$_4$ channels:C$_2$H$_2$+iC$_4$H$_5$→fulvene→C$_6$H$_5$CH$_2$ isomers→C$_6$H$_6$. The C$_4$+C$_5$ pathway: CH$_3$+C$_5$H$_5$→C$_5$H$_5$CH$_3$→(fulvene and C$_6$H$_5$CH$_2$ radicals)→C$_6$H$_6$ tends to be the dominant route for benzene formation at temperatures above 1000K. In addition to the present data, the model predicts well ignition delay times reported in literature.
New Method and Software for Computer-Aided Flowsheet Design and Analysis

Process synthesis-design involves identification of the best processing route to produce a desired product from a specified set of raw materials. In this work a systematic, multistage method and corresponding software (ProCAFD) is developed for sustainable process synthesis-design and analysis of chemical and biochemical processes. The developed method is capable of generating all the alternatives for a synthesis problem covering the entire search space of alternatives. The synthesis method is based on a group contribution based hybrid approach, where chemical process flowsheets are synthesized in the same way as atoms or groups of atoms are synthesized to form molecules in computer aided molecular design (CAMD) techniques. Another important aspect of this method is the integration of economic, sustainability and LCA analyses in the early stages of process synthesis to identify process hotspots and further improve the process using innovative design strategies. An overview of the key concepts and the method is presented along with a case study to generate sustainable designs for production of benzene from toluene and hydrogen.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Auburn University
Authors: K. Tula, A. (Ekstern), Gani, R. (Intern), Eden, M. R. (Ekstern)
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Conference: 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 01/10/2017 - 01/10/2017
New pentose dimers with bicyclic moieties from pretreated biomass
In lignocellulosic biorefinery processes involving enzyme catalysed reactions it is a challenge that enzyme inhibiting compounds are generated and liberated during pretreatment of the biomass. In this study the contribution to cellulase inhibition from xylooligosaccharides and newly discovered oligophenolic compounds from pilot scale pretreated wheat straw was assessed at two different pretreatment severities. An increase in severity of the pretreatment led to more oligophenol compounds and in turn the total overall cellulase inhibition increased. When the xylooligosaccharides were enzymatically degraded prior to cellulose hydrolysis, a relief in cellulase inhibition was observed, but some inhibition remained, suggesting that other components also played a role in inhibition. We propose that these components include dipentoses with bicyclic moieties and feruloylated tripentoses, because LC-MS/MS analysis revealed the presence of these components in the liquid from hydrothermal pretreated wheat straw after enzymatic treatment. The reaction mechanisms for synthesis of the new dipentoses having hydroxylated oxane bicyclic residues are considered and they are proposed to be formed as reaction products from either xylose or glucose reacting with glyceraldehyde during pretreatment. The data show that the main cellulase inhibition from hydrothermally pretreated wheat straw liquors is due to xylooligosaccharides followed by oligophenolic compounds and the newly discovered dipentose with bicyclic moieties and feruloylated tripentoses. The relative amounts and hence contribution to inhibition from each class of compounds changes with severity of the pretreatment.

General information
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Organisations: Department of Chemistry, Organic Chemistry, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DONG Energy A/S
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Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Web of Science (2016): Indexed yes
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Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
ISI indexed (2012): ISI indexed no
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Noncatalytic Direct Liquefaction of Biorefinery Lignin by Ethanol

There is a growing interest in lignin valorization to biofuels and chemicals. Here, we propose a novel and simple noncatalytic process to directly liquefy lignin rich solid residual from second generation bioethanol production by solvolysis with ethanol. Through an extensive parameter study in batch autoclaves assessing the effects of varying reaction temperature, reaction time, and solvent:lignin ratio, it is shown that hydrothermally pretreated enzymatic hydrolysis lignin solvolysis in supercritical ethanol can produce a heptane soluble bio-oil without the need for exhaustive deoxygenation. The process does not require addition of catalyst or a reducing agent such as hydrogen. The process is advantageously carried out with a low reaction period (<1 h) and with a reduced amount of solvent to lignin feedstock (ethanol:lignin (w/w) ratio of 2:1) which is a previously unexplored domain for lignin solvolysis. The resulting bio-oil product is mainly a mixture of di- and monomeric lignin species where the original lignin unit linkages have been broken. The oxygen content is lowered to <10 wt % (corresponding to an HHV of 36 MJ/kg) and the bio-oil is stable and acid free (verified by NMR), and due to the use of sulfur free lignin rich residual as feedstock, the resulting oil product is equally sulfur free. The residual solid product (char) has a reduced oxygen content relative to the lignin feed and equally increased higher heating value, making it a candidate for use as a biochar.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Danish Polymer Centre, University of Copenhagen
Authors: Nielsen, J. B. (Intern), Jensen, A. (Ekstern), Madsen, L. R. (Intern), Larsen, F. H. (Ekstern), Felby, C. (Ekstern), Jensen, A. D. (Intern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Indexed yes
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Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Non-linear Shear and Uniaxial Extensional Rheology of Polyether-Ester-Sulfonate Copolymer Ionomer Melts

We present unique nonlinear shear and extensional rheology data of unentangled amorphous polyester ionomers based on polyethers and sulphonated phthalates with sodium/ lithium counterions. Previous linear viscoelastic (LVE) measurements showed significant elasticity in these ionomers due to formation of strong ionic aggregates. These ionomer melts exhibit viscoelastic properties similar to well-entangled melts with an extended rubbery plateau. To evaluate the effects of nonlinear deformation, the rheology of these ionomers was investigated using uniaxial extension and shear. The measurements were performed on an updated filament stretching rheometer and on a strain controlled shear rheometer equipped with a cone-partitioned-plate (CPP) setup. In extension, ionomer samples exhibited a decreasing strain hardening trend with increasing extension rates. The presence of high solvating poly (ethylene oxide) (PEO) along the backbone in the coionomer with poly (tetramethylene glycol) PTMO, increases the maximum Hencky strain at fracture thus adding ductility to the brittle PTMO-Na ionomer. As a result, the coionomer deforms much more compared to PTMO-Na but both fracture eventually. On the other hand, whereas PTMO-Na cannot be sheared due to slip at the wall, the coionomer deforms in shear and eventually suffers from edge fracture instabilities. From the above, a picture emerges suggesting that PEO coionomers enhance ductility, make fracture smoother and offers a compromise of mechanical performance and ion conduction.

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Numerical simulation of scale-up effects of methanol-to-olefins fluidized bed reactors

Scale-up of fluidized bed reactors has long been regarded as a big challenge in chemical reaction engineering. While traditional scaling theories are mostly based on hydrodynamics similarity, computational fluid dynamics (CFD) aided approach allows direct coupling between hydrodynamics and reaction factors and is expected to speed up the experiment-based scale-up process with lower cost. In this study, we aim to investigate the scale-up effects through simulations of a
series of methanol-to-olefins (MTO) reactors of different sizes. The two-fluid model and energy-minimization multi-scale (EMMS)-based drag models are combined in simulations. The fluidization characteristics in terms of flow structures, velocity distribution, mass fractions of gaseous product and coke distribution are presented against available experimental data for different-sized reactors. It is found that typical hydrodynamic features can be reasonably predicted, while the prediction of reaction behavior shows growing discrepancy with increasing reactor size. Possible reasons are discussed in the last section along with future work presented for scale-up studies.
On a novel strategy for water recovery and recirculation in biorefineries through application of forward osmosis membranes

A great amount of research has been performed during the last 10 years focusing on forward osmosis (FO) processes. The main driving force is to find an effective and low energy demanding methodology for water recovery as well as up-concentration of valuable products. Nevertheless, the energetic and financial benefits of this technology can be undermined from the fact that FO should be usually coupled with reverse osmosis (RO) for subsequent water purification and draw solution regeneration. Hence, a different approach was applied in order to omit the RO step. Crude glycerol and enzymatically pretreated wheat straw, which are common 2nd generation biorefinery feedstocks, have been evaluated as possible draw solution. In this way, water can be directly recovered and transferred back into the fermentation loop without further purification. Applying the Aquaporin Inside™ Forward Osmosis system, crude glycerol and wheat straw hydrolysate have demonstrated water fluxes up to 10.5 L/m²/h and 5.37 L/m²/h, respectively. Furthermore, economic analysis of FO coupled with bioprocessing has demonstrated that substantial financial cost reduction regarding the product recovery can be achieved. All in all, this novel approach can be applied for both water recovery and up-concentration of soluble products in the fermentation broth and presents a great potential within biorefineries.
On the link between nonlinear extensional rheology and morphology of polymeric fibers

The mechanical properties of semi-crystalline polymeric products are highly dependent on morphology obtained during processing. For example, an ultra-high modulus polyethylene fiber owes its strength to the formation of extended chain crystals rather than folded chain crystals during fiber spinning. The imposed rate of deformation along with the molecular architecture of the polymer determines the extent of molecular deformation in the flow and which, in turn, dictates the morphology of the final product. Rheology, commonly known as “the study of flow”, can link molecular architecture to the final morphology. While numerous experimental investigations on the effect of shear flow on crystallization and the final morphology of semicrystalline materials exists, analogous studies performed in extension are much more limited. This is due to experimental difficulties that only recently have been resolved with development of the filament stretching rheometer.

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Wingstrand, S. L. (Intern), Hassager, O. (Intern), Szabo, P. (Intern)
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Operating considerations of ultrafiltration in enzyme enhanced carbon capture

Today, enzyme enhanced carbon capture and storage (CCS) is gaining interest, since it can enable the use of energy efficient solvents, and thus potentially reduce the carbon footprint of CCS. However, a limitation of this technology is the high temperatures encountered in the stripper column, which can deactivate the enzymes. One solution to this challenge is the use of ultrafiltration to retain the enzyme in the absorber unit. In this report, a base case of a CCS facility is used to model the impact of such membranes for use in a full scale CCS commercial plant. The base case has an approximate capture capacity of 1 MTonn CO2/year, and is here operated for one year continuously. This publication compares soluble enzymes dissolved in a capture solvent with and without the use of ultrafiltration membranes. The membranes used here have an enzyme retention of 90%, 99% and 99.9%. Enzyme retention is the amount of enzyme that is retained in the absorption column in each cycle. These membranes were modeled with five stripper temperatures 60 °C, 70 °C, 80 °C, 90 °C and above 100 °C. Enzyme deactivation follows a 1st order rate and increases with increasing temperatures. It was found that for all stripper temperatures used in this model, deactivation rates were too high for continuous operation over 1 year, without adding additional enzyme, if an activity of at least 50% should be maintained. With increasing stripper temperatures the membrane retention requirement increased. To retain over 50% activity over a whole year at 70 °C stripper temperature required a membrane of 90% or higher enzyme retention, at stripper temperatures of 90 °C a membrane of 99.9% retention was required for the same result. Finally, it was investigated if stripper temperatures over 100 °C, where instant deactivation was modeled could be used. It was found that with enzyme retention of 99.9%, with instant deactivation, after 1 month 50% of the activity is lost. Thus the use of membranes in enzyme enhanced CCS might be restricted to temperatures below 100 °C, or temperatures the enzyme can withstand for shorter time periods.

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Optimal design and planning of glycerol-based biorefinery supply chains under uncertainty

The optimal design and planning of glycerol-based biorefinery supply chains is critical for the development and implementation of this concept in a sustainable manner. To achieve this, a decision-making framework is proposed in this work, to holistically optimize the design and planning of the glycerol-based biorefinery supply chains under uncertainties. This framework presents a multi-layered strategy composed of different steps, and it is strongly based on optimization techniques, detailed economic and environmental assessment, and multi-objective optimization under a stochastic environment. To maximize the business value, the economic objective is measured by the Net Present Value (NPV), whereas the environmental performance is measured by the estimation of a Single Indicator (SI) through the application of LCA methods. As part of the framework, a stochastic multi-period, multi-product and multi-echelon mixed integer linear programming problem is proposed based upon a previous model, GlyThink. In the new formulation, market uncertainties are taken into account at the strategic planning level. The robustness of the supply chain structures is analyzed based on statistical data provided by the implementation of the Monte Carlo method, where a deterministic optimization problem is solved for each scenario. Furthermore, the solution of the stochastic multi-objective optimization model, points to the Pareto set of trade-off solutions obtained when maximizing the NPV and minimizing environmental consequences. Therefore, the proposed framework ultimately leads to the identification of the optimal design and planning decisions for the development of environmentally conscious biorefinery supply chains. The effectiveness of the presented approach is demonstrated through its application to the realistic case study of the glycerol-based biorefinery in Europe, where the results showed that the optimal solution under market uncertainties is obtained by establishing a multiproject supply chain for the glycerol-based integrated biorefinery, built upon two plant site locations (Germany, France) based on the production of succinic acid and lactic acid.

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Optimal operation and stabilising control of the concentric heat-integrated distillation column (HIDiC)

This paper presents the application of a systematic control configuration design procedure on the HIDiC with a reboiler. The application is illustrated through two case studies of industrial relevance, namely the separation of benzene/toluene and a multicomponent mixture of aromatic compounds. Results of static optimisations and dynamic simulations are presented based on a realistic column model, which accounts for dynamic pressure drops and liquid holdups, dynamic energy balances and more. Using a decentralised control scheme, good stabilising and economic performance are achieved by controlling both column section pressures and the temperature profile in one of the sections, while the economic variables are controlled by cascade control loops. Guidelines for the design of both the regulatory control layer and the supervisory control layer are provided.
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Authors: Bisgaard, T. (Intern), Skogestad, S. (Ekstern), Abildskov, J. (Ekstern), Huusom, J. K. (Intern)
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Optimisation of Silicone-based Dielectric Elastomer Transducers by Means of Block Copolymers - Synthesis and Compounding

Emerging artificial muscle technology has developed from metal-based robotics to soft-type robotics made from soft matter. Research into artificial muscle technology based on soft matter has been conducted mainly in order to mimic soft and robust human muscle. In this regard, dielectric elastomers have been studied. Their actuation occurs when Maxwell stress exceeds elastic stress in the presence of an electrical field, resulting in contraction in thickness and planar expansion in the area. As well as an actuator, dielectric elastomers can be used as generators and sensors. As a dielectric elastomer, silicones have been used extensively in many applications, due to favourable properties such as thermal stability, non-conductivity, high gas permeability and low toxicity. However, silicones have a low dielectric constant and thereby low energy density. In order to enhance actuation performance, it is the aim of this research to develop silicone elastomers with a high dielectric constant and high electrical breakdown strength, as well as a low Young's modulus.

In this Ph.D. thesis, two methods were developed to enhance silicone properties such as the dielectric constant and electrical breakdown strength. The first method was devised to enhance the dielectric constant of silicone elastomers through the use of a polydimethylsiloxane-polyethyleneglycol (PDMS-PEG) copolymer, in order to obtain an elastomer with high electrical energy. PDMS-PEG copolymers were synthesised and blended in commercial silicone and subsequently cross-linked. The relative permittivity of cross-linked silicone with 5 wt% of PDMS-PEG copolymers increased by nearly 50%, without compromising dielectric loss and mechanical properties, compared to the commercial silicone elastomer.

The second investigated method involved enhancing the electrical breakdown strength of silicone by using an aromatic voltage stabiliser. Here, polyphenylmethylsiloxane (PPMS), which contained aromatic voltage stabilisers, was bonded covalently to PDMS through a hydrosilylation reaction obtaining PDMS-PPMS copolymers. The synthesised copolymers were subsequently cross-linked with a vinyl cross-linker. The obtained cross-linked PDMS-PPMS copolymers were inherently soft and robust with increased electrical breakdown strength (21%) compared to the reference elastomer without an aromatic voltage stabiliser.

The conducting polymer was developed through the use of a multi-walled carbon nanotube (MWCNT) in a PDMS-PEG matrix as a compliant electrode of dielectric elastomers. The conductive PDMS-PEG copolymer was incorporated with surface-treated MWCNT, in order to obtain highly conductive elastomer. The prepared sample with 4 parts per hundred rubber (phr) MWCNT was soft and the resulting conductivity of the cross-linked PDMS-PEG copolymer with the addition of MWCNT was high, at 10-2 S cm-1, nearly equivalent to a commonly used commercial conducting polymer.

In this thesis, the elastomer and electrode system is referred to as a ‘dielectric elastomer transducer.’
Optimising and Predicting Performance of Industrial Filtrations using Process Data

Industrial cake filtration is non-trivial from an operational point of view. Discrete events such as the removal of filter cake occur on a frequent but irregular basis. These events tend to upset the steady state of the incorporating line, which may constrain plantwide optimisation. A case study has been carried out with an industrial partner where changes in the biological feedstock act as strong disturbances on a series of manually reinitialised dead-end pressure leaf filters. This renders production planning a challenging task which, so far, is carried out by experienced operators. We look for shortcomings in the current, heuristically grown manner of operating the filters and present guidelines for a superior strategy. A predictive process model is required for a deterministic scheduling algorithm, and two approaches at modelling the filtrations are presented and compared.

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Optimization-based design of waste heat recovery systems

Today, a large portion of the products that are vital to sustainability of our society are chemical products. These products have a wide range of applications within healthcare, medicine, agriculture, food, plastics and industrial processes. Therefore, chemical product development is regarded as one of the most important areas of chemical engineering today. The process efficiency and sustainability, in a considerable number of applications, depends on an array of chemical products. To ensure efficient, safe and environmental friendly processes, new chemical products need to be designed and/or selected. This dissertation focuses on the chemical product and process systems used for waste heat recovery. Here, chemical products are working fluids, which are under continuous development and screening to fulfill regulatory environmental protection and safe operation requirements. Furthermore, for the recovery of low-grade waste heat, new fluids and processes are needed to make the recovery technically and economically feasible. As the chemical product is influential in the design of the process system, the design of novel chemical products must be considered with the process system. Currently, state-of-the-art computer-aided design methods can only inadequately design novel chemical products and processes as they are considered separately and independently. Heuristics and know-how can provide feasible alternatives, but requires much user interruption, many resources and can only consider few candidates. Other than working fluids, the thesis presents other product types and applications of relevance, including solvent design.

In this thesis, a holistic framework is presented for the design of novel chemical products as a means of process systems design. The framework ensures optimal design of the chemical product and process system in terms of efficiency and sustainability. Today, some of the most important chemical product design problems are solvents and working fluids. Solvents are a vital part in the recovery of valuable resources in separation processes or waste water treatment. Working fluids are needed for the recovery of industrial waste heat and in refrigeration, air conditioning and engines, where many fluids today are phasing out due to regulative measures. The developed framework can design new chemical products, as demonstrated in cases of working fluid and solvent design, with the optimal design of the process system it is applied in. The framework requires the input of the chemical product and process needs, which through a set of systematic steps and
Flexible multi-generation systems (FMGs) consist of integrated and flexibly operated facilities that provide multiple links between the different sectors of the energy system. The present study treated the design optimization of a conceptual FMG which integrated a methanol-producing biorefinery with an existing combined heat and power (CHP) unit and industrial energy utility supply in the Danish city of Horsens. The objective was to optimize economic performance and minimize total CO₂ emission of the FMG while it was required to meet the local district heating demand plus the thermal utility demand of the butchery. The design optimization considered: Selection, dimensioning, location and integration of processes; operation optimization with respect to both hourly variations in operating conditions over the year as well as expected long term energy system development; and uncertainty analysis considering both investment costs and operating conditions. Applying a previously developed FMG design methodology, scalable models of the considered processes were developed and the system design was optimized with respect to hourly operation over the period 2015–2035. The optimal design with respect to both economic and environmental performance involved a maximum-sized biorefinery located next to local industry rather than in connection with the existing CHP unit. As the local industry energy demands were limited when compared to the biorefinery dimensions considered, process integration synergies were found to be marginal when compared to the economic and environmental impact of the biorefinery for the present case.

Assessing the impact of uncertainties on the estimated FMG performances, the net present value (NPV) of the optimal design was estimated to vary within the range 252.5–1471.6 M€ in response to changes of ± 25% in investment costs and methanol price, and considering two different electricity price scenarios. In addition, a change in the interest rate from 5% to 20% was found to reduce the lower bound of the NPV to 181.3 M€ for reference operating conditions. The results suggest that the applied interest rate and operating conditions, in particular the methanol price, would have a much higher impact on the economic performance of the designs than corresponding uncertainties in investment costs. In addition, the
study outcomes emphasize the importance of including systematic uncertainty analysis in the design optimization of FMG concepts.
Optimization of Aqueous Ammonia Soaking of manure fibers by Response Surface Methodology for unlocking the methane potential of swine manure

Swine manure mono-digestion often results to economically non-feasible processes, due to the high dilution and ammonia concentration together with the low degradation rates it presents. The effects of different parameters of Aqueous Ammonia Soaking (AAS) as a pretreatment for improving the digestion of manure fibers when coupled to an ammonia removal step were investigated in this study. Response Surface Methodology was followed and the influence and interactions of the following AAS parameters were studied: NH3 concentration, duration and solid-to-liquid ratio. The mild conditions found to be optimal (7% w/w NH3, 96 hours, and 0.16 kg/l) in combination to a significant increase of the short term CH4 yield (244% in 17 days), make this pretreatment a promising solution for improving swine manure mono-digestion. Furthermore, compositional analysis of the manure fibers revealed significant solubilization of hemicellulose, while no lignin removal or loss of cellulose occurred under optimal conditions.
Optimization Techniques for Improving the Performance of Silicone-Based Dielectric Elastomers

Dielectric elastomers are possible candidates for realizing products that are in high demand by society, such as soft robotics and prosthetics, tactile displays, and smart wearables. Diverse and advanced products based on dielectric elastomers are available; however, no elastomer has proven ideal for all types of products. Silicone elastomers, though, are the most promising type of elastomer when viewed from a reliability perspective, since in normal conditions they do not undergo any chemical degradation or mechanical ageing/relaxation. Within this review, different pathways for improving the electro-mechanical performance of dielectric elastomers are highlighted. Various optimization methods for improved energy transduction are investigated and discussed, with special emphasis placed on the promise each method holds. The compositing and blending of elastomers are shown to be simple, versatile methods that can solve a number of optimization issues. More complicated methods, involving chemical modification of the silicone backbone as well as controlling the network structure for improved mechanical properties, are shown to solve yet more issues. From the analysis, it is obvious that there is not a single optimization technique that will lead to the universal optimization of dielectric elastomer films, though each method may lead to elastomers with certain features, and thus certain potentials.
Optimizing catalytic deoxygenation of biomass derived fast pyrolysis vapors

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Oxidation of lignin in hemp fibres by laccase: effects on mechanical properties of hemp fibres and unidirectional fibre/epoxy composites

Laccase activity catalyzes oxidation and polymerization of phenols. The effect of laccase treatment on the mechanical properties of hemp fibres and hemp fibre/epoxy composites was examined. Laccase treatment on top of 0.5% EDTA + 0.2% endo-polygalacturonase (EPG) treatments increased the mechanical properties of hemp fibres and fibre/epoxy composites. Comparing all fibre treatments, composites with 0.5% EDTA + 0.2% EPG + 0.5% laccase treated fibres had highest stiffness of 42 GPa and highest ultimate tensile strength (UTS) of 326 MPa at a fibre volume content of 50%. The thermal resistance of hemp fibres increased after laccase treatments, as the maximum degradation temperature increased about 5 °C. Oxidation of phenolic hydroxyls in lignin by laccase was observed. Cross-linking of hydroxycinnamates by laccase was not observed. We suggest that the increased mechanical properties of laccase treated hemp fibres and their composites were due to laccase catalyzed polymerization of lignin moieties in hemp fibres.

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Oxidative cleavage and hydrolytic boosting of cellulose in soybean spent flakes by Trichoderma reesei Cel61A lytic polysaccharide monoxygenase

The auxiliary activity family 9 (AA9) copper-dependent lytic polysaccharide monoxygenase (LPMO) from *Trichoderma reesei* (EG4; TrCel61A) was investigated for its ability to oxidize the complex polysaccharides from soybean. The substrate specificity of the enzyme was assessed against a variety of substrates, including both soy spent flake, a by-product of the soy food industry, and soy spent flake pretreated with sodium hydroxide. Products from enzymatic treatments were analyzed using mass spectrometry and high performance anion exchange chromatography. We demonstrate that TrCel61A is capable of oxidizing cellulose from both pretreated soy spent flake and phosphoric acid swollen cellulose, oxidizing at both the C1 and C4 positions. In addition, we show that the oxidative activity of TrCel61A displays a synergistic effect capable of boosting endoglucanase activity, and thereby substrate depolymerization of soy cellulose, by 27%.

General information

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Pages: 58-66
Oxygen Dependent Biocatalytic Processes
Enzyme catalysts have the potential to improve both the process economics and the environmental profile of many oxidation reactions especially in the fine- and specialty-chemical industry, due to their exquisite ability to perform stereo-, regio- and chemo-selective oxidations at ambient temperature and pressure. A significant number of enzymes carrying out redox reactions (oxidoreductases) requiring molecular oxygen as an electron acceptor – those termed oxidases, monooxygenases and dioxygenases. These enzymes catalyze a range of industrially relevant reactions, such as oxidation of alcohols to aldehydes and ketones, oxyfunctionalization of C-H bonds, and epoxidation of C-C double bonds.

Although oxygen dependent biocatalysis offers many possibilities, there are numerous challenges to be overcome before an enzyme can be implemented in an industrial process. These challenges require the combined effort of protein engineering (i.e. modification of the amino acids sequence to improve activity, stability and selectivity) and reaction engineering (i.e. modification of reaction conditions to increase the yield and productivity) to be solved. The most important reaction engineering challenge is the requirement for oxygen, because the transfer of oxygen from the gas-phase (typically air) to the aqueous phase, where the reaction takes place, is notoriously slow due to the low aqueous solubility of oxygen at ambient conditions. Therefore, vigorous agitation and aeration is required to create a large interfacial area for mass transfer, which is not only expensive but also sets a limit to the maximum productivity of the reactor. The oxygen transfer problem is further complicated by gas-liquid interface induced enzyme deactivation, large dependency of the catalytic rate on the oxygen concentration in solution and stripping of volatile organic compounds from the reaction mixture.

In this thesis, the supply of oxygen and the implications on the biocatalyst performance are studied. The important kinetics of the reaction between enzyme and oxygen are described in detail. In fact, it is found that most enzymes operate far below their potential maximum catalytic rate at industrially relevant oxygen concentrations. Detailed knowledge of the enzyme kinetics are therefore required in order to determine the best operating conditions and design oxygen supply to minimize processing costs. This is enabled by the development of the tube-in-tube reactor (TITR) setup, capable of performing fully automated kinetic characterization of oxygen dependent enzymes - at oxygen concentrations allowing full saturation of the enzyme. The development of the TITR enables us to characterize a range of enzyme variants developed through protein engineering. This not only exemplifies the importance of knowing the full enzyme kinetics when choosing an enzyme variant for further development, but also that it is in fact possible to change the oxygen reactivity of an enzyme through substitution of amino acid residues.

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Parameter estimation and analysis of an automotive heavy-duty SCR catalyst model

A single channel model for a heavy-duty SCR catalyst was derived based on first principles. The model considered heat and mass transfer between the channel gas phase and the wash coat phase. The parameters of the kinetic model were estimated using bench-scale monolith isothermal data. Validation was done by simulating the output from a full-scale SCR monolith that was treating real engine gases from the European Transient Cycle (ETC). Three simplified models were derived, with simplifications that substantially decreased simulation time. These simplified models were coupled with the kinetic model and parameters of the nominal model, and their predictive performances were compared. Based on the results, two of the models were chosen for recalibration of the kinetic parameters, and analysed again. The results show that, after recalibration, the model that included simplifications related to mass transfer was able to keep most of its predictive capabilities, while the simulation time was reduced substantially.

General information

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Peptide Pattern Recognition for high-throughput protein sequence analysis and clustering

Large collections of protein sequences with divergent sequences are tedious to analyze for understanding their phylogenetic or structure-function relation. Peptide Pattern Recognition is an algorithm that was developed to facilitate this task but the previous version does only allow a limited number of sequences as input. I implemented Peptide Pattern Recognition as a multithread software designed to handle large numbers of sequences and perform analysis in a reasonable time frame. Benchmarking showed that the new implementation of Peptide Pattern Recognition is twenty times faster than the previous implementation on a small protein collection with 673 MAP kinase sequences. In addition, the new implementation could analyze a large protein collection with 48,570 Glycosyl Transferase family 20 sequences without reaching its upper limit on a desktop computer. Peptide Pattern Recognition is a useful software for providing comprehensive groups of related sequences from large protein sequence collections.
Perspectives on Resource Recovery from Bio-Based Production Processes: From Concept to Implementation

Recovering valuable compounds from waste streams of bio-based production processes is in line with the circular economy paradigm, and is achievable by implementing "simple-to-use" and well-established process separation technologies. Such solutions are acceptable from industrial, economic and environmental points of view, implying relatively easy future implementation on pilot- and full-scale levels in the bio-based industry. Reviewing such technologies is therefore the focus here. Considerations about technology readiness level (TRL) and Net Present Value (NPV) are included in the review, since TRL and NPV contribute significantly to the techno-economic evaluation of future and promising process solutions. Based on the present review, a qualitative guideline for resource recovery from bio-based production processes is proposed. Finally, future approaches and perspectives toward identification and implementation of suitable resource recovery units for bio-based production processes are discussed.

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Phaeobacter piscinae sp. nov., a species of the Roseobacter group and potential aquaculture probiont

Four heterotrophic, antimicrobial, motile, marine bacterial strains, 27-4T, 8-1, M6-4.2 and S26, were isolated from aquaculture units in Spain, Denmark and Greece. All four strains produced the antibiotic compound tropodithietic acid, which is a key molecule in their antagonism against fish pathogenic bacteria. Cells of the strains were Gram-reaction-negative, rod-shaped and formed star-shaped aggregates in liquid culture and brown-coloured colonies on marine agar. The predominant cellular fatty acids were C18:1ω7c, C16:0, C11 methyl C18:1ω7c and C16:0 2-OH, and the polar lipids comprised phosphatidylglycerol, diphosphatidylglycerol, phosphatidylethanolamine, phosphatidylcholine, an aminolipid, a phospholipid and an unidentified lipid. The strains grew optimally at 31-33°C. Growth was observed at a salt concentration between 0.5 and 5-6% NaCl with an optimum at 2-3%. The pH range for growth of the strains was from pH 6 to 8-8.5 with an optimum at pH 7. Based on 16S rRNA gene sequence analysis, the strains are affiliated with the genus Phaeobacter. The genome sequences of the strains have a DNA G+C content of 60.1% and share an average nucleotide identity (ANI) of more than 95%. The four strains are distinct from the type strains of the closely related species Phaeobactergallaeciensis and Phaeobacterininhibens based on an ANI of 90.5-91.7 and 89.6-90.4%, respectively, and an in silico DNA-DNA hybridization relatedness of 43.9-46.9 and 39.8-41.9%, respectively. On the basis of phylogenetic analyses as well as phenotypic and chemotaxonomic properties, the isolates are considered to represent a novel species, for which the name Phaeobacter piscinae sp. nov. is proposed. The type strain is 27-4T (=DSM 103509T=LMG 29708T).

General information
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Organisations: Department of Biotechnology and Biomedicine, Bacterial Ecophysiology and Biotechnology, DTU Metabolomics Core, Natural Product Discovery, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Leibniz-Institut DSMZ
Phase Equilibrium Modeling for Shale Production Simulation

Production of oil and gas from shale reservoirs has gained more attention in the past few decades due to its increasing economic feasibility and the size of potential sources around the world. Shale reservoirs are characterized by a more tight nature in comparison with conventional reservoirs, having pore size distributions ranging in the nanometer scale. Such a confined nature introduces new challenges in the fluid phase behavior. High capillary forces can be experienced between the liquid and vapor, and selective adsorption of components onto the rock becomes relevant. The impact of these effects is of great importance to understanding the storage of hydrocarbons inside and to forecasting its production. In this thesis, a study focused on the effects of capillary pressure and adsorption on phase behavior, and their impact on oil production is provided. An efficient algorithm for phase envelope calculations in the presence of the capillary pressure is presented, and it is used to analyze the main changes on the phase boundary for several fluids of interest. The results show changes in the saturation pressure and temperature along the phase envelope, except at the critical point. A linear analysis is presented to explain such changes, as a result, useful mathematical relationships that estimate the magnitude of these changes were obtained. Moreover, a flash algorithm that accounts for capillarity was developed. The algorithm was implemented into a fully implicit compositional reservoir simulator, which was then used to assess the impact of the capillary pressure on phase behavior in oil and gas production from tight reservoirs. Since capillary pressure and adsorption occur simultaneously in shale, its combined effect was studied. A model comparison for high-pressure adsorption in shale is presented. The adsorption data in shale is generally scarce, therefore, additional capabilities besides the accuracy were considered in the comparison. The multicomponent potential theory of adsorption yields the best results. Moreover, it shows to be useful to extrapolate adsorption data for hydrocarbons that are not available in the literature. An algorithm for phase split calculations considering both capillary pressure and adsorption was developed. The results show that adsorption and capillary pressure can significantly change the phase behavior. In general, a much shrunk phase envelope with a shifted critical point is obtained for hydrocarbon mixtures. Such behavior is mainly caused by compositional changes in the bulk phase due to selective adsorption of the heavier components onto the rock, while the change in bubble point pressure is mainly due to capillary pressure. This study has developed several robust calculation tools for phase equilibrium in porous media with capillary pressure and adsorption effects. Analysis using these tools have shown that capillary pressure and adsorption have non-negligible effects on phase equilibrium in shale. As general tools, they can be used to calculate phase equilibrium in other porous media as well. The compositional simulator with added capillary pressure effects on phase equilibrium can be used for evaluating the effects in dynamic and more complex scenarios.
inoculation with arbuscular mycorrhizal fungi. The line Oh43 was identified to show superior response and, along with five other reference lines, was characterized in greater detail in a split-compartment system, using 33 P to quantify mycorrhizal phosphorus uptake. Changes in relative growth indicated variation in host capacity to profit from the symbiosis. Shoot phosphate content, abundance of root-internal and -external fungal structures, mycorrhizal phosphorus uptake, and accumulation of transcripts encoding plant PHT1 family phosphate transporters varied among lines. Superior response in Oh43 is correlated with extensive development of root-external hyphae, accumulation of specific Pht1 transcripts and high phosphorus uptake by mycorrhizal plants. The data indicate that host genetic factors influence fungal growth strategy with an impact on plant performance.

General information
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Scopus rating (2014): SJR 3.348 SNIP 2.025 CiteScore 5.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.132 SNIP 1.985 CiteScore 6.13
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 3.232 SNIP 2.029 CiteScore 5.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 3.081 SNIP 1.936 CiteScore 5.45
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.755 SNIP 1.749
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.811 SNIP 1.962
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.56 SNIP 1.898
Pilot absorption experiments with carbonic anhydrase enhanced MDEA

Mass transfer experiments were carried out on DTU's pilot absorber unit, a 10 m high column packed with 250 Y Mellapak structured packing. The influence of temperature, solvent loading, column height and liquid flow rates on absorption performance were determined for a 30 wt% N-methyl-diethanolamine (MDEA) solvent, with and without the enzyme carbonic anhydrase (CA). The absorption experiments were performed at atmospheric pressure and a gas phase carbon dioxide mole fraction of 0.13. During experiments liquid samples were withdrawn at each meter of column height and the solvent loading was determined by both a density method and the BaCl2 method. After the solvent was loaded to equilibrium it was heated up and reintroduced into the column, where CO2 was stripped off using air as stripping gas. The addition of CA increased the mass transfer significantly in all experiments. Lower absorption temperatures resulted in higher mass transfer in absorption, when 28 and 40 ºC inlet temperature were chosen. The absorption performance decreased with lower solvent flow. The enzyme was also capable of enhancing the desorption process, where higher desorption rates were measured at 45 and 50 ºC with CA enhanced solvent compared to 55 ºC without CA.

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BFI (2015): BFI-level 1
Plant Availability of Phosphorus in Five Gasification Biochars

The innovation and expansion in the bioenergy sector produce increased amounts of solid residues, e.g., ashes and biochars, which may derive from more diverse origins of biomass. Recycling of nutrients like phosphorus (P) in such residues to agricultural soils contributes to sustainability in both energy and agriculture systems. In this study, the P availability was tested in five gasification biochars (GBs) produced via a novel low-temperature (<750°C) gasification technology. The feedstocks used were wheat straw (STR), shea nut shells (NUT), poultry manure (POUL), and two types of sewage sludge mixed with wheat straw (SSA and SSB). A 16-week laboratory incubation study of the materials was conducted with three contrasting soils and resin-extractable P (available P) and pH were monitored. Another mini-plot experiment was done to examine the effects of GBs on spring barley on a loamy sand soil. Neither barley yield nor P uptake showed significant increase after application of the GBs or a mineral P fertiliser, indicating non-limiting P status in this soil and non-adverse effect on the crop growth. During the incubation, all GBs increased soil pH markedly, especially in the STR- and NUT-amended soils and in acid soils. Of the P applied in STR, NUT, and POUL 21–29% was recovered as resin-extractable P in the two acid soils after incubation, while in the alkaline soil the recovery from STR (49%) almost matched that from triple superphosphate (52%). Recoveries from SSA and SSB were similarly low (<14%). A significant positive relationship was identified between the resin-extractable P and the resulting pH in soils amended with some GBs with low P contents. These results revealed varying P availability of low-temperature GBs, which depends on the feedstock type and pH level in the soil, and it also showed a varying ability of GBs to substitute mineral P fertilisers.
Plant-wide modelling of phosphorus transformations in wastewater treatment systems: Impacts of control and operational strategies

The objective of this paper is to report the effects that control/operational strategies may have on plant-wide phosphorus (P) transformations in wastewater treatment plants (WWTP). The development of a new set of biological (activated sludge, anaerobic digestion), physico-chemical (aqueous phase, precipitation, mass transfer) process models and model interfaces (between water and sludge line) were required to describe the required tri-phase (gas, liquid, solid) compound transformations and the close interlinks between the P and the sulfur (S) and iron (Fe) cycles. A modified version of the Benchmark Simulation Model No. 2 (BSM2) (open loop) is used as test platform upon which three different operational alternatives (A1, A2, A3) are evaluated. Rigorous sensor and actuator models are also included in order to reproduce realistic control actions. Model-based analysis shows that the combination of an ammonium (SNHX) and total suspended solids (X_{TSS}) control strategy (A1) better adapts the system to influent dynamics, improves phosphate (SPO4) accumulation by phosphorus accumulating organisms (X_{PAO}) (41%), increases nitrification/denitrification efficiency (18%) and reduces aeration energy (E_{Aeration}) (21%). The addition of iron (for chemical P removal (A2)) promotes the formation of ferric oxides (X_{HFO-H}, X_{HFO-L}), phosphate adsorption (X_{HFO-H,P}, X_{HFO-L,P}), co-precipitation (X_{HFO-H,P,old}, X_{HFO-L,P,old}) and consequently reduces the P levels in the effluent (from 2.8 to 0.9 g P.m^-3). This also has an impact on the sludge line, with hydrogen sulfide production (G_{H2S}) reduced (36%) due to iron sulfide (X_{FeS}) precipitation. As a consequence, there is also a slightly higher energy production (E_{production}) from biogas. Lastly, the inclusion of a stripping and crystallization unit (A3) for P recovery reduces the quantity of P in the anaerobic digester supernatant returning to the water line and allows potential struvite (X_{MgNH4PO4}) recovery ranging from 69 to 227 kg.day^-1 depending on: (1) airflow (Q_{stripping}); and, (2) magnesium (Q_{Mg(OH)2}) addition. All the proposed alternatives are evaluated from an environmental and economical point of view using appropriate performance indices. Finally, some deficiencies and opportunities of the proposed approach when performing (plant-wide) wastewater treatment modelling/engineering projects are discussed.

General information

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University, University of Queensland, University of Cape Town, Ghent University, Universite Laval
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Polymer liquids fracture like solids
While fracture in brittle solids has been studied for centuries until today, there are few studies on fracture in polymer liquids. Recent developments in experimental techniques, especially the combination of controlled filament stretching rheometry and high speed imaging, have opened new windows into the detailed study of fracture processes for polymer liquids. High speed imaging shows that polymer liquids fracture like solids with initiation and propagation of an edge fracture. However, remarkable features such as highly reproducible critical stress, independent appearance of multiple fractures, and trumpet crack profiles, reveal mechanisms which are significantly different from solids.

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Huang, Q. (Intern), Hassager, O. (Intern)
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Post Curing as an Effective Means of Ensuring the Long-term Reliability of PDMS Thin Films for Dielectric Elastomer Applications

Post curing can be used to facilitate volatile removal and thus produce polydimethylsiloxane (PDMS) films with stable elastic and electrical properties over time. In this study, the effect of post curing was investigated for commercial silicone elastomer thin films as a means of improving long-term elastomer film reliability. The Young’s moduli and electrical breakdown strengths of commercial (silica-reinforced) PDMS elastomer films, with and without additional 35 parts per hundred rubber titanium dioxide (TiO2), were investigated after high-temperature (200°C) post curing for various time spans. The elastomers were found to contain less than 2% of volatiles (significantly higher for TiO2-filled samples), but nevertheless a strong effect from post curing was observed. The young’s moduli as well as the strain-dependent behavior were found to change significantly upon post curing treatment, where Young’s moduli at 5% strain increase with post curing. Furthermore, the determined dielectric breakdown parameters from Weibull analyses showed that greater electrical stability and reliability could be achieved by post curing the PDMS films before usage, and this method therefore paves a way toward more reliable dielectric elastomers.

General information

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
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Scopus rating (2016): SJR 0.389 SNIP 0.57 CiteScore 1.34
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.663 SNIP 1.129 CiteScore 2.52
BFI (2013): BFI-level 1
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Scopus rating (2012): SJR 0.624 SNIP 1.027 CiteScore 1.57
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.464 SNIP 0.881 CiteScore 1.26
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.335 SNIP 0.594
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.288 SNIP 0.526
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.277 SNIP 0.559
**Powder stickiness in milk drying: uncertainty and sensitivity analysis for process understanding**

A powder stickiness model based in the glass transition temperature (Gordon – Taylor equations) was built for a production scale milk drying process (including a spray chamber, and internal/external fluid beds). To help process understanding, the model was subjected to sensitivity analysis (SA) of inputs/parameters, and uncertainty analysis (UA) to estimate confidence intervals on model predictions. For SA, a differential local and also a global approach were used. A variance decomposition method (e.g. Sobol first order sensitivity index) was implemented for global SA, and Monte Carlo technique for nonlinear error propagation was selected as the main UA approach. SA results show an important local sensitivity on the spray dryer, but at the end of the internal fluid bed (critical point for stickiness) minor local sensitivities were observed. Feed concentrate moisture was found as the input with major global sensitivity on the glass transition temperature at the critical point, so it could represent a key variable for helping on stickiness control. UA results show the major model predictions uncertainty on the spray dryer, but it does not represent a stickiness issue since the product is not in contact with dryer walls. The confidence interval for the glass transition temperature at the critical point was evaluated and this will be useful for further optimization efforts under stickiness constraints.

**Practical enhancement factor model based on GM for multiple parallel reactions: Piperazine (PZ) CO₂ capture**

Reactive absorption is a key process for gas separation and purification and it is the main technology for CO₂ capture. Thus, reliable and simple mathematical models for mass transfer rate calculation are essential. Models which apply to parallel interacting and non-interacting reactions, for all industrially relevant reaction regimes must be developed and validated against experimental measurements. In a previous work, we presented the general model (GM) enhancement factor model for (m+n)-th order reversible reactions and validated it against the numerical solution of the two-film model for absorption, desorption and pinch conditions. In this work, we apply the GM model to multiple parallel reactions. We deduce the model for piperazine (PZ) CO₂ capture and we validate it against wetted-wall column measurements using 2, 5 and 8
molal PZ for temperatures between 40 °C and 100 °C and CO₂ loadings between 0.23 and 0.41 mol CO₂/2 mol PZ. We show that overall second order kinetics describes well the reaction between CO₂ and PZ accounting for the carbamate and bicarbamate reactions. Here we prove the GM model for piperazine and MEA but we expect that this practical approach is applicable for various amines, blends of amines and promoted amines with similar kinetics. We believe that this practical implementation of mass transfer rate calculation will be in the accuracy range of a wetted wall column experiment for other parallel reaction systems. This is in line with our observation from other similar solvents studied, not shown here. Furthermore, we compare the GM model and the numerical solution of the complete two-film model predictions to MEA wetted-wall data and we prove that it is safe to assume that GM and the two-film model give practically identical results. We demonstrate that the expected predictability of CO₂ mass transfer rates using off-the-shelf correlations generally is ±20%.

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Authors: Gaspar, J. (Intern), Fosbøl, P. L. (Intern)
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Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 1.319 SNIP 1.708
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.293 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.299 SNIP 1.6
Prebiotic potential of pectin and pectic oligosaccharides to promote anti-inflammatory commensal bacteria in the human colon

Dietary plant cell wall carbohydrates are important in modulating the composition and metabolism of the complex gut microbiota, which can impact on health. Pectin is a major component of plant cell walls. Based on studies in model systems and available bacterial isolates and genomes, the capacity to utilize pectins for growth is widespread among colonic Bacteroidetes but relatively uncommon among Firmicutes. One Firmicutes species promoted by pectin is Eubacterium eligens. E. eligens DSM3376 utilizes apple pectin and encodes a broad repertoire of pectinolytic enzymes, including a highly abundant pectate lyase of around 200 kDa that is expressed constitutively. We confirmed that certain Faecalibacterium prausnitzii strains possess some ability to utilize apple pectin and report here that F. prausnitzii strains in common with E. eligens, can utilize the galacturonide oligosaccharides DP4 and DP5 derived from sugar beet pectin. F. prausnitzii strains have been shown previously to exert anti-inflammatory effects on host cells, but we show here for the first time that E. eligens strongly promotes the production of the anti-inflammatory cytokine IL-10 in in vitro cell-based assays. These findings suggest the potential to explore further the prebiotic potential of pectin and its derivatives to re-balance the microbiota towards an anti-inflammatory profile.
Prediction of Gas Injection Effect on Asphaltene Precipitation Onset Using the Cubic and Cubic-Plus-Association Equations of State

Gas injection is a proven enhanced oil recovery technique. The gas injection changes the reservoir oil composition, temperature, and pressure conditions, which may result in asphaltene precipitation. In this work, we have used a modeling approach from the literature in order to predict asphaltene precipitation onset during gas injection. The modeling approach is used with the Soave Redlich Kwong, Soave Redlich Kwong-Plus-Huron Vidal mixing rule and cubic-plus-association (CPA) equations of state (EoS). Six different reservoir fluids are studied with respect to asphaltene onset precipitation during nitrogen, hydrocarbon gas mixture, and carbon dioxide injection. It is also shown how to extend the modeling approach when the reservoir fluid is split into multiple pseudocomponents. It is observed that the modeling approach using any of the three models can predict the gas injection effect on asphaltene onset conditions. The CPA EoS is more reliable than the other two models, which are sensitive to asphaltene molecular weight and sometimes predict highly nonlinear behavior outside the experimental temperature range used for fitting the model parameters.
Prediction of Pectin Yield and Quality by FTIR and Carbohydrate Microarray Analysis

Pectin production is complex, and final product quality assessment is generally accomplished at the end of the process using time-consuming off-line laboratory analysis. In this study, pectin was extracted from lime peel either by acid or by enzymes. Fourier transform infrared spectroscopy and carbohydrate microarray analysis were performed directly on the crude lime peel extracts during the time course of the extractions. Multivariate analysis of the data was carried out to predict final pectin yields. Fourier transform infrared spectroscopy (FTIR) was found applicable for determining the optimal extraction time for the enzymatic and acidic extraction processes, respectively. The combined results of FTIR and carbohydrate microarray analysis suggested major differences in the crude pectin extracts obtained by enzymatic and acid extraction, respectively. Enzymatically extracted pectin, thus, showed a higher degree of esterification (DE 82 %) than pectin extracted by acid (DE 67 %) and was moreover found to be more heterogeneously esterified when probed with the monoclonal antibodies JIM5, JIM7, and LM20. The data infer that enzymatic pectin extraction allows for extraction of complex, high DE pectin, and that FTIR and carbohydrate microarray analysis have potential to be developed into online process analysis tools for prediction of pectin extraction yields and pectin features from measurements on crude pectin extracts.
Prediction of properties of new halogenated olefins using two group contribution approaches

The increasingly restrictive regulations for substances with high ozone depletion and global warming potentials are driving the search for new sustainable fluids with low environmental impact. Recent research works have pointed out the great potential of fluorine- and chlorine-based olefins as refrigerants and solvents, due to their environmentally-friendly features. However there is a lack of experimental data of their thermophysical properties. In this work we present two models based on a group contribution method, using a classical approach and neural networks, to predict the critical temperature, critical pressure, normal boiling temperature, acentric factor, and ideal gas heat capacity of organic fluids containing chlorine and/or fluorine. The accuracy of the prediction capacity of the two models is analyzed, and compared with equivalent methods in the literature. The models showed an average reduction of the absolute relative deviation for all the studied properties of more than 50%, compared to other methods. In addition, it was observed that the neural-network-based model yielded a better accuracy than the classical approach in the prediction of all the properties, except for the acentric factor, due to the lack of experimental data for this property.

General information
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Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
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Preface

It has been a pleasure to edit this special issue on process intensification (PI), a topic that is attracting much attention from industry as well as academia. Process systems engineering (PSE) has been closely related to the developments within PI and this special issue of Computers and Chemical Engineering has collected papers from invited authors covering a wide range of topics within PI. We include the idea of any process design feature that retains the primary process objectives (production rate and fitness-for-use criteria) while also improving one or more performance parameters which could include economics (raw material consumption, energy requirement, labor requirement, other operating costs, equipment capital, working capital, etc.), environmental impacts, physical plant size, employment, flexibility, controllability, robustness, reliability, safety, etc. Topics covering synthesis issues, modelling issues, design issues, analysis issues, new application examples, process improvement, etc. are included in this special issue.

General information
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Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Purdue University
Pre-oxidation and its effect on reducing high-temperature corrosion of superheater tubes during biomass firing

Superheater tubes in biomass-fired power plants experience high corrosion rates due to condensation of corrosive alkali chloride-rich deposits. To explore the possibility of reducing the corrosion attack by the formation of an initial protective oxide layer, the corrosion resistance of pre-oxidised Al and Ti-containing alloys (Kanthal APM and Nimonic 80A, respectively) was investigated under laboratory conditions mimicking biomass firing. The alloys were pre-oxidised at 900°C for 1 week. Afterwards, pre-oxidised samples, and virgin non-pre-oxidised samples as reference, were coated with a synthetic deposit of KCl and exposed at 560°C for 1 week to a gas mixture typical of biomass firing. Results show that pre-oxidation could hinder the corrosion attack; however, the relative success was different for the two alloys. While corrosion attack was observed on the pre-oxidised Kanthal APM, the pre-oxidised Nimonic 80A remained unaffected suggesting protection of the alloy from the corrosive environment.

General information
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Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Technical University of Denmark
Authors: Okoro, S. C. (Intern), Kvisgaard, M. (Ekstern), Montgomery, M. (Intern), Jappe Frandsen, F. (Intern), Pantleon, K. (Intern)
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.29 SJR 0.406 SNIP 0.716
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.423 SNIP 0.659 CiteScore 1.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.453 SNIP 0.862 CiteScore 1.34
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.594 SNIP 0.843 CiteScore 1.54
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.619 SNIP 0.919 CiteScore 1.5
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.375 SNIP 0.752 CiteScore 0.88
ISI indexed (2011): ISI indexed yes
Pre-process desilication of wheat straw with citrate

Effects of treatment time, citrate concentration, temperature, and pH on Si extraction from wheat straw prior to hydrothermal pretreatment were investigated for maximising Si removal and biomass recovery before biomass refining. With citrate, an almost linear negative correlation between Si content in the residual biomass and treatment temperature was observed up to 170 degrees C, yielding a Si removal of up to 97.7%. This high Si removal came at the expense of a low mass yield (down to 45%) in the insoluble lignocellulosic fraction. Optimum process conditions for high Si removal and high total mass yield were: 100mM sodium citrate, 130 degrees C, 60 min, 2% w/v solids, and pH of similar to 6.5 during extraction. Using the proposed process conditions, silica removal of up to 77% was achieved with a mass yield of 72.8%. This Si removal from the insoluble lignocellulosic fraction did not affect the enzymatic cellulose hydrolysis, neither negatively nor positively.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DONG Energy A/S
Authors: Le, D. M. (Intern), Sorensen, H. R. (Ekstern), Meyer, A. S. (Intern)
Pages: 126-132
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Process Biochemistry
Volume: 55
ISSN (Print): 1359-5113
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Process assessment associated to microbial community response provides insight on possible mechanism of waste activated sludge digestion under typical chemical pretreatments

Current studies have employed various chemicals for disintegrating and hydrolyzing microbial cells in waste activated sludge (WAS). However, a comprehensive process assessment over the whole anaerobic digestion process has seldom been proposed. Besides, the characterization of microbial community responses to these chemicals is not well understood. In this study, the effects of five typical chemicals: solubilizer (β-cyclodextrin, CD), alkaline (NaOH), peroxide (peracetic-acid, PA), biological (rhamnolipid, RL) and chemical (sodium dodecylsulphate, SDS) surfactants on WAS digestion were examined. Higher efficiencies of WAS solubilization, hydrolysis and acidification were achieved by CD treatment, followed by RL and SDS. Methanogenesis was also strongly chemicals-dependent. Shifts in microbial community structure were observed in all chemical-pretreated WAS. The community in RL, CD and PA was dominated by microorganisms that anaerobically hydrolyze organics to acids, while that in NaOH and SDS was mainly associated to biogas production. This study proved that the overall performance of WAS digestion was substantially depended on the initial chemical pretreatments, which in turn influenced and was related to the microbial community structures. Although the economic advantage might not be clear yet, the findings obtained in this work may provide a scientific basis for the potential implementation of chemicals for WAS treatment.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Taiyuan University of Technology, Chinese Academy of Sciences
Pages: 457-467
Publication date: 2017
Main Research Area: Technical/natural sciences

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Journal: Energy
Volume: 137
ISSN (Print): 0360-5442
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.17 SJR 1.999 SNIP 1.798
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.276 SNIP 2.046 CiteScore 5.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.647 SNIP 2.63 CiteScore 5.7
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.54 SNIP 2.593 CiteScore 5.02
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.998 SNIP 2.25 CiteScore 4.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.609 SNIP 2.043 CiteScore 4
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.814 SNIP 2.725
Process design, supply chain, economic and environmental analysis for chemical production in a glycerol biorefinery:
Towards the sustainable design of biorefineries

Drivers such as our deep dependence on fossil fuels availability and price volatility, global concern about climate change and social distress, are steering the economy to be more sustainable and based on a greater use of renewable resources. Therefore, the concept of integrated biorefineries has attracted much attention by aspiring at replacing fossil sources. However, as has been recently witnessed through multiple failures and the shutdown of biorefinery plants all over the world, a biobased economy that heavily depends on the production of biofuels, leads to unsatisfactory results. Thus, it seems that an economy based on the innovative and cost–efficient use of bio-resources for the production of both chemicals and biofuels/bioenergy, is in fact very promising regarding the three pillars of sustainability (economic, environmental and social). Notwithstanding, to be competitive in the long run and to present an advantage in the global markets, robust systems for the acquisition, production and distribution of these bioproducts must be in place. Although considerable studies have been carried out on the analysis and optimization of biomass conversion to biofuels and bioenergy, up to date limited research has been done on the valorization of biorefinery by-products. This is especially noticeable concerning the valorization of glycerol, which is, as main by-product of the biodiesel industry, responsible for approximately 2/3 of the world supply of glycerol. Despite the many uses for pure glycerol, the exponential growth of biodiesel production in a recent past due to fossil-based energy insecurity and environmental concerns, has led to a significant surplus of glycerol, resulting in a significant drop of its market value. Then, how to deal with the large quantities of low price crude glycerol surplus may become an environmental problem. As a result, exploratory research being carried out along the years has been pointing to glycerol as a powerful starting material for the production of a plethora of value-added chemicals and biofuels. A significant challenge is that emerging technologies are accompanied by uncertain performance characteristics, as well as exogenous sources of uncertainty such as product price and demand. This leads to a significant number of possible options regarding the design, operation and product portfolio offered by biorefineries, from which the most suitable process configurations must be selected, with regards to economics, environmental constraints and overall sustainability. Therefore, uncertainties should not be overlooked. Furthermore, given the multiplicity of large (bio)chemical operations and the often-conflicting objectives among the several business divisions, such as planning, manufacturing, distribution and corresponding environmental consequences and concerns, it is therefore vital to model these activities and to develop comprehensive and systematic methods to capture the synergies and the trade-offs within this complex system. Therefore, the foremost aim of this thesis is to provide a roadmap for early-stage managerial decisions targeting at identifying feasible alternatives for the design and planning of sustainable glycerol biorefineries and corresponding value chains. In this way the thesis is contributing to the transition towards the sustainable development and implementation of these concepts. To achieve this, significant effort is firstly invested into process understanding and into the development of data-driven process models (‘gate-to-gate’). Secondly, detailed methodologies for the economic and environmental assessment are developed, where uncertainty and sensitivity analysis play a
significant role. Nevertheless, in order to further advance the development and implementation of glycerol based biorefinery concepts, it is critical to analyze the glycerol conversion into high value-added products in a holistic manner, considering both production as well as the logistics aspects related to the supply chain structure. Therefore, the boundaries of analysis were extended to include all activities and operations involved in the glycerol-based biorefinery to bioproducts supply chain. To this end, the GlyThink model is proposed so as to identify operational decisions - including locations, capacity levels, technologies and product portfolio, as well as strategic decisions such as inventory levels, production amounts and transportation to the final markets. GlyThink is a multi-period, multi-stage and multi-product Mixed Integer Linear Programming optimization model based on the maximization of the associated Net Present Value (NPV). Furthermore, strongly based upon the GlyThink model, alongside with detailed economic and environmental assessment, a multi-layered framework for the optimal design and planning of glycerol based biorefinery supply chains under uncertainties is developed in this thesis. The proposed integrated framework ultimately leads to the identification of the optimal design and planning decisions for the development of environmentally conscious biorefinery supply chains, where the consequences of external economic uncertainties on the environmental objective function are analyzed and the trade-offs identified. In summary, this thesis covers the development of methods and tools for the modeling and optimization at the strategic and tactical level, along with detailed economic and environmental assessment techniques, including the incorporation of multi-level uncertainties. All in all, despite the fact that all methods and tools derived in this thesis have been developed to address the optimal design and planning of the glycerol-based biorefinery, they are flexible and applicable to other biorefineries similar in nature.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Loureiro da Costa Lira Gargalo, C. (Intern), Sin, G. (Intern), Carvalho, A. I. C. D. S. G. (Ekstern), Gernaey, K. V. (Intern)
Number of pages: 201
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**Publication information**

Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences

**Relations**

Projects:
Process design, supply chain, economic and environmental analysis for chemical production in a glycerol biorefinery:
Towards the sustainable design of biorefineries
Source: PublicationPreSubmission
Source-ID: 134654408
Publication: Research › Ph.D. thesis – Annual report year: 2017

**Propane Oxidation at High Pressure and Intermediate Temperatures**
Propane oxidation at intermediate temperatures (500—900 K) and high pressure (100 bar) has been characterized by conducting experiments in a laminar flow reactor over a wide range of stoichiometries. The onset of fuel oxidation was found to be 600—725 K, depending on mixture stoichiometry. The model agreed well with the measurements of fuel-rich and stoichiometric mixtures while the model underpredicted the fuel conversion for fuel-lean conditions. Sensitivity analyses revealed the importance of H-abstraction reactions by HO₂, OH, and CH₃OO in controlling propaneoxidation at 750 K.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Hashemi, H. (Intern), Christensen, J. M. (Intern), Glarborg, P. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at 8th European Combustion Meeting, Dubrovnik, Croatia.
Main Research Area: Technical/natural sciences
Electronic versions: ecm2017_14_1.pdf
Publication: Research - peer-review › Poster – Annual report year: 2017

**Property Model-Based Chemical Substitution and Chemical Formulation Design**
Chemical-based products including structured product formulations and single molecule products have proven to be a boon to mankind and have been a significant part of our economies. Our life and the changes around us cannot be
imagined without the presence or involvement of chemicals. But like every coin has two sides, some chemicals
constituting these products can also be a curse. This is primarily due to the hazardous environment-related properties
that some of these chemicals possess and there are many more chemicals which have not been evaluated due to lack of
resources for rigorous, experimental-based estimation methods [1]. Hence, there is a dire necessity to identify such
chemicals which may be dangerous to the environment, toxic to human health and harmful for our fragile eco-system.

Besides, in many cases, their corresponding chemical production processes generate harmful emissions, which also have
severe impacts on the environment. The concern about the environment and human health has given rise to the REACH
regulation implemented by the European Chemical Agency (ECHA), which compels European chemical companies to stop
the use of hazardous substances and replace them with environmentally benign chemicals. Additionally, the decisions
taken during chemical product design also have an impact on the process and product performance and are influenced by
company strategy, availability of market and government policies [2]. Hence, undoubtedly there is a need to develop a
systematic, model-based methodology that can help to find substitutes to existing chemicals in order to improve process
economics, operability as well as the sustainability, while still delivering the same or improved product functionality. It is
useful to start with making structured databases by collecting data from knowledge base, followed by the development of
the predictive group-contribution property models and then the development of a general methodology for the model-
based chemical substitution and chemical product design. The objective here is to quickly and reliably identify the
promising candidates through model-based techniques and then to verify and evaluate their performance and applicability
through experiments. In this way, the experimental resources are used for verification rather than for an inefficient, trial-
and-error search used for practically all chemical products. Besides, when it is desired to come up with alternative
substitutes for the undesirable chemicals, the trial an error based approach will have a very large search space. This could
be avoided by having predictive models coupled with the desired target properties, making the identification of these
substitutes easier. The goal therefore is to investigate comprehensively the uses and properties of the chemicals of
concern; develop a systematic framework to identify, compare and select safer alternatives to these including their
corresponding manufacturing processes; and finally design safe chemical product formulations or product formulations
with improved product performance. The model-based approach makes use of validated property models to identify the
chemicals which need to be substituted, that is, the chemicals that meet the desired physico-chemical properties but not
the regulatory (EH&S: environmental, health and safety) properties, and then to generate, evaluate and identify candidates
that can replace them. The presentation will discuss the general methodology for chemical substitution, which caters to
different problem definitions depending on the reason for substitution. The associated property modeling tools [3] will also
be highlighted. A set of new group contribution-based models for a number of useful properties of amino acids will be
presented. Through examples on substitution of chemicals from chemical-based products from various sectors namely
cosmetics and personal care, pharmaceutical and food, with amino acids (as active ingredient or as additive) will be
shown along with other well-known substitution problems. These examples will also highlight the role of property models in
chemical substitution and chemical product formulation.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CERE – Center for Energy
Ressources Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre
(CoAST)
Authors: Jhamb, S. V. (Intern), Liang, X. (Intern), Hukkerikar, A. S. (Intern), Dam-Johansen, K. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2017
Event: Abstract from 2017 AIChE Annual Meeting, Minneapolis, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Property_Model.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Property Uncertainty Analysis and Methods for Optimal Working Fluids of Thermodynamic Cycles
There is an increasing interest in recovering industrial waste heat at low temperatures (70-250 °C). Thermodynamic
cycles, such as heat pumps or organic Rankine cycles, can recover this heat and transfer it to other process streams or
convert it into electricity. The working fluid, circulating around the cycle, is vital for the performance of the cycle.
Computational modelling of working fluid properties and cycle processes allows to identify promising working fluid
candidates together with optimal cycle conditions.

However, such computer simulations are subject to modelling uncertainties due to the operational conditions, process
correlations and fluid properties. In this thesis the focus lies on the uncertainties from physical and chemical property data,
caused by the experimental measurements or by the prediction models.

This thesis project presents a comprehensive framework to assess property uncertainties for different levels of
thermodynamic cycle models. The framework consists of 1) a methodology for the development and uncertainty analysis
of group contribution based property models, 2) a Bootstrap method for the quantification of uncertainties associated to
equations of state parameters, 3) a Monte Carlo procedure for the propagation of property uncertainties through the cycle
process onto the model output uncertainty, and 4) novel strategies for the selection of working fluids under property
uncertainties, in particular a new reverse engineering approach based on sampling and uncertainty concepts. The
framework is applied to different applications and case studies from industrial project partners.

Novel group contribution based property models are developed for the estimation of flammability-related properties (e.g.
the lower flammability limit) of working fluids. Compared to existing models, the ones presented here show a higher accuracy, are simpler to apply and provide every prediction value with its corresponding uncertainty range (with 95% confidence). The study also reveals that group contribution methods can suffer from parameter identifiability issues characterized by a significant correlation between estimated parameters. Hence, in order to ensure reliable estimation, reporting the 95% confidence interval of the model predictions is important.

In a second application it is shown how the uncertainty propagation of two types of equations of states, cubic and PC-SAFT, can be compared in the context of an industrial organic Rankine cycle, used for the recovery of waste heat from an engine of a marine container ship. The study illustrates that the model structure is vital for the uncertainties of equations of state and suggests that uncertainty becomes a criterion (along with e.g. goodness-of-fit or ease of use) for the selection of an equation of state for a specific application.

Furthermore, two studies on the identification of suitable working fluids for thermodynamic cycles are presented. The first one selects and assesses working fluid candidates for an organic Rankine cycle system to recover heat from a low-temperature heat source. The ranking of working fluids can be significantly different based whether the mean value or the uncertainties (e.g. the lower bound of the 95%-confidence interval) of the model output are considered. Hence, uncertainty analysis with respect to the input property uncertainties is a vital tool for model analysis and fluid selection.

In the second fluid selection study the novel reverse engineering approach based on sampling techniques and uncertainty analysis is applied to identify suitable working fluids for a industrial heat pump system, used to recover heat from spray-drying air in dairy industries. The novel reverse engineering approach provides a valid alternative to computationally demanding optimization approaches and allows to take into account property uncertainties.

The outcome of this thesis asserts that property uncertainties should be taken into account for process simulation applications, in order to support the model-based and reliable decisions on process fluids and process design.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre
Authors: Frutiger, J. (Intern), Sin, G. (Intern), Abildskov, J. (Ekstern)
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Electronic versions:
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Relations
Projects:
Property Uncertainty Analysis and Methods for Optimal Working Fluids of Thermodynamic Cycles
Publication: Research › Ph.D. thesis – Annual report year: 2017

Prospects of the use of nanofluids as working fluids for organic Rankine cycle power systems
The search of novel working fluids for organic Rankine cycle power systems is driven by the recent regulations imposing additional phase-out schedules for substances with adverse environmental characteristics. Recently, nanofluids (i.e. colloidal suspensions of nanoparticles in fluids) have been suggested as potential working fluids for organic Rankine cycle power systems due to their enhanced thermal properties, potentially giving advantages with respect to the design of the components and the cycle performance. Nevertheless, a number of challenges concerning the use of nanofluids must be investigated prior to their practical use. Among other things, the trade-off between enhanced heat transfer and increased pressure drop in heat exchangers, and the impact of the nanoparticles on the working fluid thermophysical properties, must be carefully analyzed. This paper is aimed at evaluating the prospects of using nanofluids as working fluids for organic Rankine cycle power systems. As a preliminary study, nanofluids consisting of a homogenous and stable mixture of different nanoparticles types and a selected organic fluid are simulated on a case study organic Rankine cycle unit for waste heat recovery. The impact of the nanoparticle type and concentration on the heat exchangers size, with respect to the reference case, is analyzed. The results indicate that the heat exchanger area requirements in the boiler decrease around 4 % for a nanoparticle volume concentration of 1 %, without significant differences among nanoparticle types. The pressure drop in the boiler increases up to 18 % for the same nanoparticle concentration, but this is not found to impact negatively the pump power consumption.

General information
State: Published
Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, KT Consortium, Technical University of Denmark, Fondazione Politecnico di Milano
Publisher's Note to Modeling the influence of potassium content and heating rate on biomass pyrolysis [Appl. Energy J. 184 (2017) 199–211]

The authors and the editors regret to report that the following errors were found in the article after its availability online.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Agder, Massachusetts Institute of Technology, Lulea University of Technology
Authors: Trubetskaya, A. (Ekstern), Surup, G. (Ekstern), Shapiro, A. (Intern), B. Bates, R. (Ekstern)
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Main Research Area: Technical/natural sciences

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Journal: Applied Energy
Volume: 202
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.854 SNIP 3.108 CiteScore 5.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.473 SNIP 2.84 CiteScore 5.5
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Deposit formation in utility boilers occurs via a number of consecutive steps; 1) release of critical elements like K, Na, Pb, Zn, S and Cl, 2) formation of gaseous species, fly ash and aerosols, 3) transport and adhesion of ash species, 4) deposit build-up and consolidation, and, finally, 5) shedding of deposits. Some of the steps may be repetitive, as the process is partly cyclic [Frandsen, 2011]. The inorganic fraction of solid fuels, may cause several problems during combustion, most importantly formation of particulate matter (aerosols and fly ashes). These may subsequently induce deposit formation (slagging and fouling) on superheater tubes, leading to a potential reduction in heat transfer efficiency to the water/steam cycle, or, to chemical attack (corrosion) or physical wear (erosion) of superheater tubes. These problems may give rise to irregular operation, or even costly shutdowns of combustion units. Through several years, high quality research has been conducted on characterization of fuels, ashes and deposit formation in utility boilers fired with coal, biomass and waste fractions. Huge amounts of experimental data have been reported, from such work, but the fact is that there are still in 2017, a number of big gaps in our current understanding of these phenomena, and that we need focus on these points, in order to be able to describe, understand, and, quantify the processes of ash and deposit formation completely [Frandsen, 2009]. This paper provide a brief outline of the current status on release of critical ash-forming elements, formation of aerosols respectively fly ash formation is systems fired with solid fuels. The paper is a significantly updated, but condensed version of a review-paper on the same subject, presented in Lapland, Northern Finland in 2010 [Frandsen et al., 2010].
Quantitative analysis of pigment dispersion taking into account the full agglomerate size distribution

This work concerns the development of simulation tools for mapping of pigment dispersion. Focus has been on the mechanical breakage of pigment agglomerates. The underlying physical mechanism was assumed to be surface erosion of spherical pigment agglomerates, and the full agglomerate particle size distribution was simulated. Data from previous experimental investigations with organic pigments were used for model validation. When the linear rate of agglomerate surface erosion was taken to be proportional to the external agglomerate surface area, simulations of the volume-moment mean diameter over time were in good quantitative agreement with experimental data. The only adjustable parameter used was an apparent rate constant for the linear agglomerate erosion rate. Model simulations, at selected values of time, for the full agglomerate particle size distribution were in good qualitative agreement with measured values. The general applicability of the model, beyond the pigments considered, needs to be confirmed.

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST)
Authors: Kiil, S. (Intern)
Number of pages: 4
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Main Research Area: Technical/natural sciences
Electronic versions: Abstract_COSI_2017_S_ren_Kiil_.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Quantitative risk assessment via uncertainty analysis in combination with error propagation for the determination of the dynamic Design Space of the primary drying step during freeze-drying

Traditional pharmaceutical freeze-drying is an inefficient batch process often applied to improve the stability of biopharmaceutical drug products. The freeze-drying process is regulated by the (dynamic) settings of the adaptable process parameters shelf temperature $T_s$ and chamber pressure $P_c$. Mechanistic modelling of the primary drying step allows the computation of the optimal combination of $T_s$ and $P_c$ in function of the primary drying time. In this study, an uncertainty analysis was performed on the mechanistic primary drying model to construct the dynamic Design Space for the primary drying step of a freeze-drying process, allowing to quantitatively estimate and control the risk of cake collapse (i.e., the Risk of Failure (RoF)). The propagation of the error on the estimation of the thickness of the dried layer $L_{dried}$ as function of primary drying time was included in the uncertainty analysis. The constructed dynamic Design Space and the predicted primary drying endpoint were experimentally verified for different RoF acceptance levels (1%, 25%, 50% and 99% RoF), defined as the chance of macroscopic cake collapse in one or more vials. An acceptable cake structure was only obtained for the verification runs with a preset RoF of 1% and 25%. The run with the nominal values for the input variables (RoF of 50%) led to collapse in a significant number of vials. For each RoF acceptance level, the experimentally determined primary drying endpoint was situated below the computed endpoint, with a certainty of 99%, ensuring sublimation was finished before secondary drying was started. The uncertainty on the model input parameters demonstrates the need of the uncertainty analysis for the determination of the dynamic Design Space to quantitatively estimate the risk of batch rejection due to cake collapse.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Ghent University
Authors: Van Bockstal, P. J. (Ekstern), Mortier, S. T. F. (Ekstern), Corver, J. (Ekstern), Nopens, I. (Ekstern), Gernaey, K. V. (Intern), De Beer, T. (Ekstern)
Pages: 32-41
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: European Journal of Pharmaceutics and Biopharmaceutics
Volume: 121
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Rate-based modelling and validation of a pilot absorber using MDEA enhanced with carbonic anhydrase (CA)

The great paradox of the 21st century is that we must meet the increasing global demand for energy and products while simultaneously mitigating the climate change. If both these criteria are to be met, carbon capture and storage is an imperative technology for sustainable energy infrastructure development. Post-combustion capture is a mature capture technology; however, to make it economically attractive, design of innovative solvents and process optimization is of crucial importance. An example for promising solvent is MDEA enhanced with carbonic anhydrase (CA), due to its fast kinetics and low solvent-regeneration energy demand. The focus of this work is to develop a rate-based model for CO2 absorption using MDEA enhanced with CA and to validate it against pilot-scale absorption experiments. In this work, we compare model predictions to measured temperature and CO2 concentration profiles for different L/G ratios, lean CO2 loadings, gas CO2 content and packing height. We show that the developed model is suitable for CO2 capture simulation.
and optimization using MDEA and MDEA enhanced with CA. Furthermore, we investigate the accuracy of the General Method (GM) enhancement factor model for CO₂ absorption/desorption using wetted-wall column data: 0 to 0.5 CO₂ loading and temperatures between 298 and 328 K. The present study represents a first step towards developing and optimizing a CA promoted MDEA CO₂ capture process.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS
Authors: Gaspar, J. (Intern), Gladis, A. (Intern), Woodley, J. (Intern), Thomsen, K. (Intern), von Solms, N. (Intern), Fosbøl, P. L. (Intern)
Pages: 707 – 718
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

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- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.16 SJR 0.467 SNIP 0.586
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.365 SNIP 0.561 CiteScore 0.92
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.433 SNIP 0.81 CiteScore 1.09
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.425 SNIP 0.785 CiteScore 1.02
- ISI indexed (2013): ISI indexed no
- Web of Science (2013): Indexed yes
- Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
- ISI indexed (2012): ISI indexed no
- Web of Science (2012): Indexed yes
- Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
- ISI indexed (2011): ISI indexed no
- Scopus rating (2010): SJR 0.433 SNIP 0.957
- Web of Science (2009): Indexed yes

Original language: English
CO₂ post-combustion capture, GM enhancement factor, Enzyme kinetics, Multiple reversible reactions, Model validation

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**Reaction Equilibrium of the ω-Transamination of (S)-Phenylethylamine: Experiments and ePC-SAFT Modeling**

This work focuses on the thermodynamic equilibrium of the ω-transaminase-catalyzed reaction of (S)-phenylethylamine with cyclohexanone to acetophenone and cyclohexylamine in aqueous solution. For this purpose, the equilibrium concentrations of the reaction were experimentally investigated under varying reaction conditions. It was observed that the temperature (30 and 37 °C), the pH (between pH 7 and pH 9), as well as the initial reactant concentrations (between 5 and 50 mmol·kg⁻¹) influenced the equilibrium position of the reaction. The position of the reaction equilibrium was moderately shifted toward the product side by either decreasing temperature or decreasing pH. In contrast, the initial ratio of the reactants showed only a marginal influence on the equilibrium position. Further experiments showed that increasing the initial reactant concentrations significantly shifted the equilibrium position to the reactant side. In order to explain these
effects, the activity coefficients of the reacting agents were calculated and the activity-based thermodynamic equilibrium
constant $K_{th}$ of the reaction was determined. For this purpose, the activity coefficients of the reacting agents were
modeled at their respective experimental equilibrium concentrations using the equation of state electrolyte PC-SAFT
ePC-SAFT). The combination of the concentrations of the reacting agents at equilibrium and their respective activity
coefficients provided the thermodynamically consistent equilibrium constant $K_{th}$. Unexpectedly, the experimental Km
values deviated by a factor of up to four from the thermodynamic equilibrium constant $K_{th}$. The observed concentration
dependency of the experimental Km values could be explained by the influence of concentration on activity coefficients.
Further, these activity coefficients were found to be strongly temperature dependent, which is important for the
determination of standard enthalpy of reactions, which in this work was found to be $+7.7 \pm 2.8 \text{ kJ mol}^{-1}$. Using the so-
determined $K_{th}$ and activity coefficients of the reacting agents (ePC-SAFT), the equilibrium concentrations of the reaction
were predicted for varying initial reactant concentrations, which were found to be in good agreement with the experimental
behavior. These results showed a non-negligible influence of the activity coefficients of the reacting agents on the
equilibrium position and, thus, on the product yield. Experiments and ePC-SAFT predictions showed that the equilibrium
position can only be described accurately by taking activity coefficients into account.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technische Universität
Dortmund
Authors: Voges, M. (Ekstern), Abu, R. (Intern), Deslauriers, M. G. (Intern), Held, C. (Ekstern), Woodley, J. (Intern),
Sadowski, G. (Ekstern)
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Publication information
Journal: Organic Process Research and Development
Volume: 21
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Ratings:
BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.48 SJR 1.062 SNIP 0.859
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.318 SNIP 1.029 CiteScore 2.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 0.99 CiteScore 2.38
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.13 SNIP 0.977 CiteScore 2.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.185 SNIP 1.12 CiteScore 2.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.212 SNIP 0.914 CiteScore 2.22
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.114 SNIP 0.97
Reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite: a combined DFT/experimental study

The reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite was studied theoretically with periodic density functional theory calculations including dispersion forces and experimentally in a fixed bed flow reactor at pressures between 10 and 100 bar, dimethyl ether concentrations in CO between 0.2 and 2.0%, and at a temperature of 438 K. The theoretical study showed that the reaction of CO with surface methyl groups, the rate-limiting step, is faster in the eight-membered side pockets than in the twelve-membered main channel of the zeolite; the subsequent reaction of dimethyl ether with surface acetyl to form methyl acetate was demonstrated to occur with low energy barriers in both the side pockets and in the main channel. The present analysis has thus identified a path, where the entire reaction occurs favourably on a single site within the side pocket, in good agreement with previous experimental studies. The experimental study of the reaction kinetics was consistent with the theoretically derived mechanism and in addition revealed that the methyl acetate product inhibits the reaction - possibly by sterically hindering the attack of CO on the methyl groups in the side pockets.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS, SLAC National Accelerator Laboratory
Authors: Rasmussen, D. B. (Intern), Christensen, J. M. (Intern), Temel, B. (Ekstern), Studt, F. (Ekstern), Moses, P. (Ekstern), Rossmeisl, J. (Intern), Riisager, A. (Intern), Jensen, A. D. (Intern)
Number of pages: 12
Pages: 1141-1152
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Main Research Area: Technical/natural sciences

Publication information
Journal: Catalysis Science & Technology
Volume: 7
Issue number: 5
ISSN (Print): 2044-4753
Ratings:
BFI (2018): BFI-level 2
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BFI (2017): BFI-level 1
Reaction of Sulfuric Acid in Lube Oil: Implications for Large Two-Stroke Diesel Engines

Slow-steaming operation and an increased pressure in the combustion chamber have contributed to increased sulfuric acid (H$_2$SO$_4$) condensation on the cylinder liners in large two-stroke marine diesel engines, thus causing increased corrosion wear. To cope with this, lube oils are formulated with overbased detergent additives present as CaCO$_3$ reverse micelles to neutralize the condensing H$_2$SO$_4$. In this present work, a mixed flow reactor (MFR) setup aims to investigate the neutralization reaction by varying Ca/S molar ratio, stirrer speed, H$_2$SO$_4$ inlet concentration, and residence time. Lube oil samples from the outlet of the MFR were analysed by use of Fourier Transform Infrared Spectroscopy (FTIR) and a titration method. The MFR results indicate that the CaCO$_3$-H$_2$SO$_4$ reaction is very fast in a real engine, if the cylinder liner is well-wetted, the oil-film is well-mixed, and contains excess of CaCO$_3$ compared to the condensed H$_2$SO$_4$. The observed corrosion wear in large two-stroke marine diesel engines could consequently be attributed to local molar excess of H$_2$SO$_4$ compared to CaCO$_3$ reverse micelles on the cylinder liners.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), MAN Diesel & Turbo SE
Authors: Lejre, K. H. (Intern), Kiil, S. (Intern), Glarborg, P. (Intern), Christensen, H. (Ekstern), Mayer, S. (Ekstern)
Number of pages: 10
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Host publication information

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Publisher: American Society of Mechanical Engineers
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ISBN (Electronic): 978-0-7918-5831-8
Main Research Area: Technical/natural sciences
Conference: Internal Combustion Engine Fall Technical Conference (ICEF 2017), Seattle, United States, 15/10/2017 - 15/10/2017
Corrosion, Lubrication, Neutralization, Mechanism
DOIs: 10.1115/ICEF2017-3580
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Recent Advances and Challenges towards Sustainable Polyhydroxyalkanoate (PHA) Production

Sustainable biofuels, biomaterials, and fine chemicals production is a critical matter that research teams around the globe are focusing on nowadays. Polyhydroxyalkanoates represent one of the biomaterials of the future due to their
physicochemical properties, biodegradability, and biocompatibility. Designing efficient and economic bioprocesses, combined with the respective social and environmental benefits, has brought together scientists from different backgrounds highlighting the multidisciplinary character of such a venture. In the current review, challenges and opportunities regarding polyhydroxyalkanoate production are presented and discussed, covering key steps of their overall production process by applying pure and mixed culture biotechnology, from raw bioprocess development to downstream processing.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Universidade Nova de Lisboa, Swansea University, University of Southampton
Authors: Kourmentza, C. (Ekstern), Plácido, J. (Ekstern), Venetsaneas, N. (Ekstern), Burniol Figols, A. (Intern), Varrone, C. (Intern), Gavala, H. N. (Intern), Rei, M. A. M. (Ekstern)
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Main Research Area: Technical/natural sciences

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Journal: Journal of Bioscience and Bioengineering
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.32 SJR 0.733 SNIP 0.951
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.71 SNIP 0.909 CiteScore 2.13
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.742 SNIP 0.933 CiteScore 2.05
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.734 SNIP 0.947 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.732 SNIP 0.957 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.726 SNIP 0.926 CiteScore 1.97
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.747 SNIP 0.992
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.788 SNIP 0.984
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.839 SNIP 1.159
Scopus rating (2007): SJR 0.662 SNIP 0.823
Scopus rating (2006): SJR 0.592 SNIP 0.775
Scopus rating (2005): SJR 0.474 SNIP 0.693
Scopus rating (2004): SJR 0.549 SNIP 0.664
Scopus rating (2003): SJR 0.498 SNIP 0.709
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.49 SNIP 0.694
Recent advances in extensional rheology: controlled flows and fracture

Extensional deformation and flow occur in a number of polymer processing operations such as fiber spinning and film blowing. To understand and analyze material behavior in such operations, accurate and quantitative measurements of the rheological properties in well-defined extensional deformations are needed. However, while shear flows may in principle easily be generated in geometries such as cone-and-plate and plate-and-plate, the generation of controlled extensional flows has proven to be a challenge [1]. This presentation will focus on the application of Filament Stretching Rheometry (FSR) to measure extensional flow properties of polymeric liquids. It will be demonstrated, that the FSR technique enables measurements in start-up of constant extensional rate flow to sufficiently large Hencky strain so that steady flow is attained for several polymer systems. In addition the FSR may be used to study the relaxation of stress after cession of flow and the transient extensional creep under conditions of constant stress. Combination of the FSR technique with other methods gives further possibilities. For example high speed imaging may be used to study and analyze crack profiles under filament fracture [2]. Likewise the deuterium labeling of selected molecules in combination with the FSR allows for the study of molecular relaxation by small angle neutron scattering [3].

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Hassager, O. (Intern), Huang, Q. (Intern)
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Release and transformation of chlorine and potassium during pyrolysis of KCl doped biomass

The formation of CH$_3$Cl and the transformation of chlorine and potassium during pyrolysis of biomass were investigated. Model biomass compounds (cellulose, xylan, lignin and pectin) and pine wood doped with KCl were pyrolysed in a TGA at different heating rates (10–1000 °C/min), temperatures (300–850 °C), and KCl contents (0–5 wt%). The volatiles were collected and analyzed for CH$_3$Cl concentration by GC–MS. The solid residue was analyzed by ICP-OES for the contents of total and water soluble K and Cl. Considerable amounts of CH$_3$Cl, corresponding to 20–50% of the fuel chlorine, were formed in pyrolysis of KCl doped pine wood, lignin and pectin samples, suggesting a methylation ability of these biomass on KCl by their methoxyl groups. Lignin and pine wood could supply methoxyl groups for reaction with as much as about 2% KCl doping, and pectin had an even greater capacity. Organic K was found in the solid residue of all samples, further supporting the occurrence of reactions between KCl and the organic matrix in biomass. With a holding temperature of 500 °C, an increase of heating rate from 10 °C/min to 500 °C/min significantly reduced the yield of CH$_3$Cl from KCl doped wood/lignin/pectin, while no further reduction effect was observed at 1000 °C/min. For a heating rate of 500 °C/min, an increase of holding temperature from 300 °C to 850 °C caused a decreased yield of CH$_3$Cl.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, North China Electric Power University
Authors: Wang, Y. (Intern), Wu, H. (Intern), Sárossy, Z. (Intern), Dong, C. (Ekstern), Glarborg, P. (Intern)
Pages: 422-432
Publication date: 2017
Main Research Area: Technical/natural sciences

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Journal: Fuel
Volume: 197
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.9 SJR 1.744 SNIP 2.179
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.809 SNIP 2.125 CiteScore 4.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.667 SNIP 2.331 CiteScore 4.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.811 SNIP 2.595 CiteScore 4.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.852 SNIP 2.465 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.093 SNIP 2.427 CiteScore 4.1
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.984 SNIP 2.319
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.012 SNIP 2.277
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.635 SNIP 2.184
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.383 SNIP 1.86
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.278 SNIP 1.64
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.623 SNIP 1.73
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.273 SNIP 1.883
Scopus rating (2003): SJR 1.103 SNIP 1.481
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.13 SNIP 1.301
Scopus rating (2001): SJR 1.136 SNIP 1.264
Scopus rating (2000): SJR 1.047 SNIP 1.272
Web of Science (2000): Indexed yes
A simple model for binary liquid–liquid equilibrium data correlation is explored. The model describes liquid–liquid equilibrium in terms of Henry’s law and unsymmetrically normalized activity coefficients in each phase. A procedure for parameter estimation including an approach to initial guesses, uncertainty analysis of regression results, obtained parameters, and predicted mole fractions has been formulated. The procedure is applied to three cases: hydrocarbons + water, ionic liquids + water, and nitroethane + hydrocarbons. The model has four parameters in the most basic formulation. Depending upon the available data, this number can be extended in a systematic fashion. We compare results of correlation to results obtained with a four-parameter nonrandom two-liquid (NRTL) equation and COSMO-SAC. In general, the new model does nearly as well as NRTL. Advantages of the presented model are a simple form and a parameter set that can be extended in a systematic fashion with an interpretation in terms of thermodynamic properties. The model may be developed further for validation of experimental data.
A presence of carbonyl compounds is very common in the food industry. The nature of such compounds is to be reactive and thus many products involve aldehydes/ketones in their synthetic routes. By contrast, the high reactivity of carbonyl compounds could also lead to formation of undesired compounds, such as genotoxic impurities. It can therefore be important to remove carbonyl compounds by implementing suitable removal techniques, with the aim of protecting final product quality. This work is focused on benzaldehyde as a model component, studying its removal from a water/ethanol mixture by applying different derivatization agents as the scavengers. Discovery chemistry is performed in the beginning as a screening procedure, followed by the process design of a small-scale continuous process for benzaldehyde removal with in-line real-time monitoring. Applications of tris(hydroxymethyl) aminomethane (TRIS) are found to provide above average removal of benzaldehyde.

### General information

**State:** Published  
**Organisations:** Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Copenhagen  
**Authors:** Mitic, A. (Intern), Skov, T. (Ekstern), Gernaey, K. V. (Intern)  
**Number of pages:** 9  
**Pages:** 353-361  
**Publication date:** 2017  
**Main Research Area:** Technical/natural sciences

### Publication information

**Journal:** Green Processing and Synthesis  
**Volume:** 6  
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**Ratings:**  
Web of Science (2018): Indexed yes  
Web of Science (2017): Indexed Yes
Reply to "Comment on 'Reliable Correlation for Liquid–Liquid Equilibria outside the Critical Region’"

We respond to the comments by Glass and Mitsos regarding our approach to validation of binary liquid–liquid equilibrium data.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, University of Virginia
Authors: Ruszczyński, Ł. (Intern), Zubov, A. (Intern), O’Connell, J. P. (Ekstern), Abildskov, J. (Ekstern)
Pages: 4043–4044
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 62
Issue number: 11
ISSN (Print): 0021-9568
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
Resource recovery from bio-based production processes: a future necessity?

The promise of transforming waste streams with small economic value into valuable products makes resource recovery technologies in bio-based production processes an attractive proposition. However, the use of resource recovery technologies in industrial applications is still minimal, despite its wide use in closely related processes such as dairy production. In this paper, a perspective on the role of resource recovery in bio-based production processes is provided through reviewing the past practice and identifying the benefits, opportunities and challenges of introducing resource recovery technologies to industrial bio-based production processes. The role and importance of economics, technology readiness and socio-environmental impacts of resource recovery in successfully implementing resource recovery technologies in industrial bio-based production processes is also discussed. Finally, based on the insights gained in this review and assessment of resource recovery technologies in the domain of bio-based production processes, an informed opinion and perspective is provided. The current state of resource recovery and the shortcomings when developing practical resource recovery applications in bio-based production processes are discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Mansouri, S. S. (Intern), S.B.A. Udugama, I. (Intern), Cignitti, S. (Intern), Mitic, A. (Intern), Flores Alsina, X. (Intern), Gernaey, K. (Intern)
Pages: 1-9
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Current Opinion in Chemical Engineering
Volume: 18
ISSN (Print): 2211-3398
Ressourcegenvinding – vejen til øget bæredygtighed i biobaserede produktionsprocesser

Reverse osmosis for water purification and reuse in the biotechnological industry: Process design, operation and economic guidelines
In this work, a generic hierarchical computer-aided framework for techno-economic assessment of resource recovery plants for biotechnological process streams is proposed. The framework consists of five main steps that can evaluate, develop and implement a resource recovery project from concept to implementation through the systematic analysis of economic potential, technology availability and readiness as well as comprehensive net present value analysis. The application of the framework is demonstrated through a case study from the biotechnological industry where the objective was to reduce the hydraulic load on a wastewater treatment plant (WWTP), thereby investigating opportunities for process water reuse. In this case, a recovery unit is studied, where purification and concentration generates large volumes of wastewater. Reverse osmosis (RO) could ensure that the desired drinking water quality could be achieved and would enable re-use of the water in the production site for different economic purposes.
Rheological Link Between Polymer Melts with a High Molecular Weight Tail and Enhanced Formation of Shish-Kebabs

Presence of an ultra high molecular weight (UHMw) fraction in flowing polymer melts is known to facilitate formation of oriented crystalline structures significantly. The UHMw fraction manifests itself as a minor tail in the molar mass distribution and is hardly detectable in the canonical characterization methods. In this study, alternatively, we demonstrate how the nonlinear extensional rheology reveals to be a very sensitive characterization tool for investigating the effect of the UHMw-tail on the structural ordering mechanism. Samples containing a UHMw-tail relative to samples without, exhibit a clear increase in extensional stress that is directly correlated with the crystalline orientation of the quenched samples. Extensional rheology, particularly, in combination with linear creep measurements, thus, enables the conformational evolution of the UHMw-tail to be studied and linked to the enhanced formation of oriented structures.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, California Institute of Technology, University of Copenhagen, University of Crete
Authors: Wingstrand, S. L. (Intern), Shen, B. (Ekstern), Kornfield, J. A. (Ekstern), Mortensen, K. (Ekstern), Parisi, D. (Ekstern), Vlassopoulos, D. (Ekstern), Hassager, O. (Intern)
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Volume: 6
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Scopus rating (2016): CiteScore 6.03 SJR 2.744 SNIP 1.307
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.407 SNIP 1.427 CiteScore 5.91
Scopus rating (2014): SJR 2.484 SNIP 1.616 CiteScore 5.66
Scopus rating (2013): SJR 2.156 SNIP 1.24 CiteScore 5.15
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Rheological properties of agar and carrageenan from Ghanaian red seaweeds

Red seaweeds contain unique galactose-rich hydrocolloids, carrageenans and agar, which find use as gelling agents in high value applications. This study examined the chemical and rheological properties of hydrocolloids from selected wild red seaweed species collected in Ghana: Hypnea musciformis and Cryptonemia crenulata, expected to hold carrageenan, contained 21–26% by weight of galactose. A commercial Kappaphycus alvarezi carrageenan sample had 30% galactose residues by weight. Hydropuntia dentata, expected to contain agar, contained 15% by weight of galactose-monomers. Fourier transform infrared spectroscopy (FTIR) analysis on the hydrocolloids extracted from H. musciformis (and K. alvarezi) indicated κ-carrageenan, C. crenulata hydrocolloids were mainly ι-carrageenan, and the H. dentata hydrocolloids were agar. Gelling temperatures ranged from 32 to 36 °C for the κ-carrageenan hydrocolloid samples. The ι-carrageenan and agar samples had gelling temperatures of 70–74 °C and 38–52 °C, respectively. Gel strengths, G' at 25 °C, of carrageenan samples extracted via alkali-treatment were 4000–6500 Pa. The agar gel strength was 287 Pa. The rheological properties of the H. musciformis κ-carrageenans were comparable with κ-carrageenan from K. alvarezi, whereas the H. dentata agar properties were different from those of a commercial agar sample. This work shows that certain red seaweed species in Ghana contain hydrocolloids with desirable properties for high value applications.

General information

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, National Food Institute, Research Group for Nano-Bio Science, The Danish Polymer Centre
Authors: Rhein-Knudsen, N. (Intern), Ale, M. T. (Intern), Ajalloueian, F. (Intern), Yu, L. (Intern), Meyer, A. S. (Intern)
Pages: 50-58
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Food Hydrocolloids
Volume: 63
ISSN (Print): 0268-005X
Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.1 SJR 2.043 SNIP 2.041
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.846 SNIP 1.966 CiteScore 4.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.251 SNIP 2.564 CiteScore 5.21
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.1 SNIP 2.292 CiteScore 4.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.866 SNIP 2.086 CiteScore 3.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
We have previously shown that galacto-rhamnogalacturonan fibers can be enzymatically extracted from potato pulp and that these fibers have potential for exerting a prebiotic effect in piglets. The spore-forming Bacillus species are widely used as probiotics in feed supplements for pigs. In this study, we evaluated the option for further functionalizing Bacillus feed supplements by selecting strains possessing the enzymes required for extraction of the potentially prebiotic fibers. We established that it would require production and secretion of pectin lyase and/or polygalacturonase but no or limited secretion of galactanase and β-galactosidase. By screening a library of 158 Bacillus species isolated from feces and soil, we demonstrated that especially strains of Bacillus amyloliquefaciens, Bacillus subtilis, and Bacillus mojavensis have the necessary enzyme profile and thus the capability to degrade polygalacturonan. Using an in vitro porcine gastrointestinal model system, we revealed that specifically strains of B. mojavensis were able to efficiently release galacto-rhamnogalacturonan from potato pulp under simulated gastrointestinal conditions. The work thus demonstrated the feasibility of producing prebiotic fibers via a feed containing Bacillus spores and potato pulp and identified candidates for future in vivo evaluation in piglets.

General information
State: Published
Organisations: Department of Biotechnology and Biomedicine, Infection Microbiology, Novo Nordisk Foundation Center for Biosustainability, Research Groups, Bacterial Signal Transduction, National Veterinary Institute, Bacteriology & Parasitology, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Chr. Hansen A/S
Authors: Jers, C. (Intern), Strube, M. L. (Intern), Cantor, M. D. (Ekstem), Nielsen, B. K. K. (Ekstem), Sørensen, O. B. (Ekstem), Boye, M. (Intern), Meyer, A. S. (Intern)
Pages: 3605-3615
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Microbiology and Biotechnology
Volume: 101
Issue number: 9
ISSN (Print): 0175-7598
Ratings:
Separation and recovery of intracellular betacarotene using a process synthesis framework

In this work, the process synthesis problem for the bio-manufacturing of high-value intracellular compounds is addressed using a systematic framework that allows for the user to input key process parameters from literature or experiments. The framework is based on a superstructure optimization approach and integrates various methods and tools, including a generic model and a database for data management (Bertran et al., 2017). We propose the following five steps: (1) problem formulation, (2) data collection and superstructure generation, (3) solution of the optimization problem, and (4) sensitivity analysis and (5) experimentation with informed design and then determination of the optimal process design. The framework is implemented in Super-O, software which guides the user through the formulation and solution of synthesis problems. This paper demonstrates the proposed framework though an illustrative case study on the production of beta-carotene from recombinant Saccharomyces cerevisiae (SM14) via continuous cultivation.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Pages: 327-335
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Pages: 327-335
Publication date: 2017
Main Research Area: Technical/natural sciences
Sequential electrodialytic recovery of phosphorus from low-temperature gasification ashes of chemically precipitated sewage sludge

Phosphorus recycling from secondary materials like sewage sludge ashes offers an alternative to mining of phosphates from primary resources and a mean to counteract the current phosphorous rock depletion concern. A separation of P from the bulk ash is normally required, due to its low plant availability and the presence of heavy metals. Previously, more than 80% of P was recovered from incineration sewage sludge ashes using a two-compartment electrodialytic cell. In contrast, the recovery was below 30% for ashes from low-temperature gasification using the same setup. The low recovery was due to a high presence of Al- and Fe(III)-P bindings. In the present study, an electrodialytic process combining sequentially a pair of two-compartment cells allowed a recovery of up to 70% of phosphorus from these ashes. The use of a second cell, where the ash was suspended in an alkaline solution, allowed the P solubilisation from aluminium and ferric phosphates. In addition, P was separated from most metals as they became insoluble under the prevailing chemical environment. The obtained ratio of Al, Fe, Mg and most heavy metals to P was comparable to wet process phosphoric acid. Therefore, this sequential process was found to be suitable to recycle P and potentially use it in the production of common fertilizers like diammonium phosphate.

General information
State: Published
Organisations: Department of Civil Engineering, ARTEK, Section for Arctic Engineering and Sustainable Solutions, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Roskilde University
Pages: 211–218
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Waste Management
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ISSN (Print): 0956-053x
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4 SJR 1.354 SNIP 2.044
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.739 SNIP 2.256 CiteScore 4.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.777 SNIP 2.482 CiteScore 3.43
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.822 SNIP 2.435 CiteScore 3.39
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.611 SNIP 2.184 CiteScore 2.91
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.698 SNIP 2.085 CiteScore 2.99
Shape optimization as a tool to design biocatalytic microreactors

Reactor design is commonly constrained to already well-known reactor shapes. This article presents an innovative application of shape optimization techniques to design biocatalytic microreactors. Currently, the optimization of reactor performance is often done by considering solely the process conditions. However, common reactor types used in (bio)chemical processes do not always give the optimal conditions for executing the reaction, and it is therefore necessary to look into new approaches to further improve the performance of reactors. The new application of shape optimization described in this paper has as its main goal the design of a reactor by compensating for the limitations of the reaction system by modifying the reactor configuration. Random search was the optimization method chosen for transforming the initial reactor configuration to a more optimal one. The case study presented here investigates the impact of a change to the microreactor shape on the active mixing of two parallel streams (one containing an enzyme, amino transaminase, and the other the substrates, acetophenone and isopropylamine) and consequently its influence on the reaction yield. Compared to the original reactor configuration, the shape optimization resulted in changes of the microreactor wall surfaces leading to an 8.4 fold improvement of the reactor yield. This innovative optimization also offers the opportunity to obtain new structures which can later be tested experimentally.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, The Danish Polymer Centre
Authors: Pereira Rosinha Grundtvig, I. (Intern), Daugaard, A. E. (Intern), Woodley, J. (Intern), Gernaey, K. (Intern), Krühne, U. (Intern)
Pages: 215–223
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Significance of membrane bioreactor design on the biocatalytic performance of glucose oxidase and catalase: Free vs. immobilized enzyme systems

Membrane separation of xylose and glucose can be accomplished via oxidation of glucose to gluconic acid by enzymatic glucose oxidase catalysis. Oxygen for this reaction can be supplied via decomposition of hydrogen peroxide by enzymatic catalase catalysis. In order to maximize the biocatalytic productivity of glucose oxidase and catalase (gluconic acid yield per total amount of enzyme) the following system set-ups were compared: immobilization of glucose oxidase alone; co-immobilization of glucose oxidase and catalase; glucose oxidase and catalase free in the membrane bioreactor. Fouling-induced enzyme immobilization in the porous support of an ultrafiltration membrane was used as strategy for entrapment of glucose oxidase and catalase. The biocatalytic productivity of the membrane reactor was found to be highly related to the oxygen availability, which in turn depended on the reactor configuration, hydrogen peroxide concentration and catalase origin. When glucose oxidase and catalase (from Aspergillus niger) were free in the membrane bioreactor a total biocatalytic productivity of 122 mg gluconic acid/mg enzyme was obtained after five consecutive reaction cycles. The free enzymes showed superior performance compared to the immobilized systems as a result of limited substrate and product...
diffusion in the latter case.

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**Publication information**

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Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 3.16
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): CiteScore 2.75
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): CiteScore 2.72
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): CiteScore 3.03
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): CiteScore 3.15
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): CiteScore 2.95
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Web of Science (2008): Indexed yes
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- Web of Science (2003): Indexed yes
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Original language: English

Biocatalytic productivity, Catalase, Fouling-induced enzyme immobilization, Glucose oxidase, Polydopamine

**DOIs:**

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Publication: Research - peer-review › Journal article – Annual report year: 2016
Silicone-based Dielectric Elastomers

Efficient conversion of energy from one form to another (transduction) is an important topic in our daily lives, and it is a necessity in moving away from the fossil based society. Dielectric elastomers hold great promise as soft transducers, since they are compliant and light-weight amongst many favorable properties. Their transduction principle lies in direct conversion of electrical energy into mechanical energy or vice versa with no need for gearing and with no stand-by energy consumption. This should in principle support a more efficient use of energy, a hot topic in our current society where energy efficient solutions are highly sought. These properties allow for interesting products ranging very broadly, e.g. from eye implants over artificial skins over soft robotics to huge wave energy harvesting plants. All these products utilize the inherent softness and compliance of the dielectric elastomer transducers.

The subject of this thesis is improvement of properties of silicone-based dielectric elastomers with special focus on design guides towards electrically, mechanically, and electromechanically reliable elastomers. Strategies for improving dielectric elastomer performance are widely investigated but rarely discussed in the context of mechanical integrity and thus product reliability. Focus here is on long-term reliability of the dielectric elastomers and how to achieve this by means of careful elastomer design. This thesis presents methods and results of analyses acquired in the cross-disciplinary, collaborative effort on dielectric elastomers funded by Innovationsfonden Denmark (formerly Advanced Technology Foundation) with the materials workgroup headed by the author. Main contributors to the work have been research scientists at Danfoss PolyPower, colleagues from the Danish Polymer Centre, as well as 7 PhD students and 5 postdocs being involved in the project. International collaborators were also part of the project at various stages. The studies behind this thesis have been conducted over a period of about 5 years, and 10 selected papers describing the main results are included as appendices. They were chosen to represent the prime results obtained within the project. Most of the technical aspects discussed in this thesis are contained within these references. Several other important works have been omitted in the appendices in order to keep the thesis relatively short and concise.

Throughout the thesis the articles within the appendices are referred to as A1-A10. For all of these articles, the author was the principal investigator. Other dielectric-elastomer related papers by the author - either as a principal investigator or co-investigator- are referred to as A11-A51. Chapters 1 to 5 of the thesis present a coherent summary of the included papers in a common context, emphasizing the overall purpose and flow of the analysis thematically. Unpublished work is included as well to facilitate coupling between approaches as well as to provide the full, comprehensive story. Chapter 6 gives a conclusion, and in Chapter 7 a personal perspective on the future of dielectric elastomer research is given.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Skov, A. L. (Intern)
Number of pages: 278
Publication date: 2017

Silicone elastomers with covalently incorporated aromatic voltage stabilisers

When optimising dielectric elastomers (DEs) a conflict exists, namely that for large achievable actuation strains softness is required, but with increased softness electrical breakdown strength decreases. Herein, soft dielectric silicone elastomers with increased electrical breakdown strength, due to the incorporation of an aromatic voltage stabiliser, were prepared by cross-linking synthesised polydimethylsiloxane–polyphenylmethylsiloxane (PDMS–PPMS) copolymers. PPMS possesses voltage stabilisation capabilities but is immiscible in PDMS, and thus the copolymerisation of the two components was necessary for homogeneity. Concentrations of the voltage stabiliser were varied by changing the molecular weights of the PPMS in the copolymer. The developed elastomers were inherently soft with enhanced electrical breakdown strengths, due to delocalised p-electrons of the aromatic constituent. An optimum concentration was found for the voltage stabilisation effect. The relative permittivities of the PDMS–PPMS elastomers varied from 3.4 to 3.9 and therefore were also improved from pure PDMS elastomers. The elastomers were furthermore non-conductive and possessed low dielectric losses. These properties are evaluated as favourable for soft actuation.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: A Razak, A. H. (Intern), Skov, A. L. (Intern)
Pages: 468-477
Publication date: 2017
Main Research Area: Technical/natural sciences
Simultaneous Description of Activity Coefficients and Solubility with eCPA

In the many developments of electrolyte equations of state presented over the past decades, several different properties have been in focus. A property that has not been widely used as a fitting property is salt solubility. This work presents a new parametrization of the eCPA equation of state with salt specific parameters. The focus is on accurate description of the salt solubility, and low deviation correlations are obtained for all salts investigated. The inclusion of the solubility data in the parametrization has, compared to parameters only parametrized to osmotic coefficients and activity coefficients, not significantly affected the deviations of the osmotic coefficients and activity coefficients. The average deviations of the activity coefficient does increase slightly and it was found that the increase in deviations was almost entirely due to reduced accuracy at high temperature and high molality. The model is, furthermore, compared to the activity coefficient model, Extended UNIQUAC. It is shown that the eCPA provides more accurate solubility description at higher temperatures than Extended UNIQUAC but also that Extended UNIQUAC is slightly better at describing the activity coefficients. Overall the two models perform similarly.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Schlaikjer, A. (Intern), Thomsen, K. (Intern), Kontogeorgis, G. (Intern)
Pages: 1074-1089
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 56
Simultaneous measurement of temperature and humidity with microstructured polymer optical fiber Bragg gratings

A microstructured polymer optical fiber (mPOF) Bragg grating sensor system for the simultaneous measurement of temperature and relative humidity (RH) has been developed and characterized. The sensing head is based on two in-line fiber Bragg gratings recorded in a mPOF. The sensor system has a root mean square deviation of 1.04 % RH and 0.8 °C in the range 10 to 90% RH and 20 to 80 °C. The proposed sensor system is easy to fabricate, cheap and compact.

Soft and flexible conductive PDMS/MWCNT composites

Conductive elastomers based on MWCNT in polydimethylsiloxane (PDMS) have been prepared by a range of dispersion methods such as ultrasonication, speedmixing and roll milling in combination with physical or covalent modification. The ionic liquid (IL), 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide, was used to pre-disperse MWCNT in a MWCNT/IL-gel that was used for preparation of MWCNT/PDMS composites. The method was seen to be effective at low levels of MWCNT, but required combination with a roll mill to obtain a stable dispersion at 4 wt % MWCNT. With higher amounts of MWCNT a reduction in conductivity was observed, which was attributed to a change in morphology occurring between 4 and 5 wt % MWCNT. As an alternative to IL dispersing aids a novel functionalized MWCNT was prepared by free radical polymerization using α-methacryloxypropyl-polydimethylsiloxane, which could be used directly for preparation of MWCNT/PDMS composites. Composites prepared by use of the IL dispersion method, use of a roll mill or by use of the f-MWCNT all had conductivities around 0.005–0.01 s/cm and retained conductivity upon extension.
Solid oxide fuel cells powered by biomass gasification for high efficiency power generation

Increased use of bioenergy is a very cost-effective and flexible measure to limit changes in the climate and the infrastructure. One of the key technologies toward a higher implementation of biomass is thermal gasification, which enables a wide span of downstream applications. In order to improve efficiencies, flexibility and possibly costs of current biomass power generating systems, a power plant concept combining solid oxide fuel cells (SOFC) and gasification is investigated experimentally. The aim of the study is to examine the commercial operation system potential of these two technologies. Investigations are done by combining the commercial TwoStage Viking gasifier developed at the Technical University of Denmark and a state-of-the-art SOFC stack from Topsoe Fuel Cell for high efficiency power generation. A total of 5 tests were performed including polarization tests at various gas flows to study part-load operation; and a longer test to investigate stability. The study shows experimentally the potential and feasibility of a SOFC-gasification system with a commercial gasifier and a SOFC stack by measuring the highest reported values of such a system, with biomass-to-electricity efficiencies up to 43%. Results from related modeling studies are also presented, showcasing the intriguing potential of the system with modeled cycle electric efficiencies up to 62%.
Solubility Modeling of the Systems Ni(NO₃)₂–H₂O and Fe(NO₃)₃–Ni(NO₃)₂–H₂O with the Extended Universal Quasichemical (UNIQUAC) Model

Thermodynamic modeling of the binary systems Ni(NO₃)₂–H₂O and Ni(NO₃)₂–H₂O and of the ternary system of Fe(NO₃)₃–Ni(NO₃)₂–H₂O along the 30 °C isotherm are presented. The extended UNIQUAC model was applied for the thermodynamic assessment of the investigated systems, the model parameters were regressed simultaneously using the available databank but with additional experimental data recently published in the open literature. A revision for previously published parameters for the nickel ion, new parameters for the iron(III) nitrate system, and interaction parameters for the Ni²⁺–Fe³⁺ interaction are presented. Based on this set of parameters, the equilibrium constants of hydrates were determined. The model represents the experimental data with good accuracy from the freezing point region to the boiling points of the solutions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University Hassan I
Authors: Arrad, M. (Ekstern), Kaddami, M. (Ekstern), El Goundali, B. (Ekstern), Thomsen, K. (Intern)
Pages: 1220–1229
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Solution Chemistry
Volume: 46
Issue number: 6
Solvent consumption in non-catalytic alcohol solvolysis of biorefinery lignin

Lignin solvolysis in supercritical alcohols provides a method for producing a deoxygenated liquid bio-oil. Solvent consumption is however inevitable and due to the high cost of alcohols, relative to a bio-oil product, it can hinder commercial viability. In order to investigate the reactions of solvent consumption we studied solvolysis of biorefinery lignin in several primary alcohols. Lignin solvolysis in methanol, ethanol, 1-propanol and 1-butanol performed similarly with respect to bio-oil composition; however, methanol gave much lower bio-oil yield. Solvent consumption increases with reaction temperature for all alcohols and from 10 wt% at 300 °C to 35 wt% at 400 °C when using ethanol. The mechanism for solvent consumption was found mainly to take place through three different reactions: direct decomposition to gas through decarbonylation, formation of light condensation products and incorporation of the alcohol into the bio-oil through
covalent bonding. Incorporation of the alcohol into the depolymerised oil product by covalent bonding may be a desirable effect which contributes to increased oil yield, inhibition of repolymerisation, reduced oxygen content and elimination of acidity.

**General information**
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Copenhagen
- **Authors:** Nielsen, J. B. (Intern), Jensen, A. (Ekstern), Schandel, C. B. (Intern), Felby, C. (Ekstern), Jensen, A. D. (Intern)
- **Pages:** 2006-2015
- **Publication date:** 2017
- **Main Research Area:** Technical/natural sciences

**Publication information**
- **Journal:** Sustainable Energy & Fuels
- **Volume:** 1
- **Issue number:** 9
- **ISSN (Print):** 2398-4902
- **Original language:** English
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- **Source:** FindIt
- **Source-ID:** 2389538080
- **Publication:** Research - peer-review › Journal article – Annual report year: 2017

**Solvolyis of Lignosulfonate Catalyzed by Supported NiMo**
Lignin is the most abundant aromatic compound on Earth. Lignin is mostly burned as a low quality fuel in pulp mills and biorefineries. Lignosulfonate is a byproduct from sulfite pulping, mainly produced by the company Borregaard [1]. Extraction of higher value products from lignosulfonate is of interest, which is rarely addressed in literature. Amongst different methods, solvothermal conversion assisted by a heterogeneous catalyst is a promising method for conversion of lignin. However, the sulfur in the structure of lignosulfonate deactivates most of the heterogeneous catalysts by sulfur deposition. Conversion of lignosulfonate to liquefied products using sulfur tolerant hydrotreating catalysts is investigated in this work.

**General information**
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS, Borregaard
- **Authors:** Ghafarnejad Parto, S. (Intern), Christensen, J. M. (Intern), Saaby Pedersen, L. (Ekstern), Taarning, E. (Ekstern), Tjosås, F. (Ekstern), Jensen, A. D. (Intern)
- **Number of pages:** 2
- **Publication date:** 2017
- **Event:** Abstract from 21st Annual Green Chemistry and Engineering Conference, Reston, United States.
- **Main Research Area:** Technical/natural sciences
- **Electronic versions:** Soheila_Parto_Abstract.pdf
- **Source:** PublicationPreSubmission
- **Source-ID:** 139905776
- **Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2017

**Solvothermal conversion of technical lignins over NiMo catalysts**
Scope: Lignin, cellulose and hemicellulose are the main constituents of plants cell walls. Lignin is an aromatic rich compound, composed of phenolic building blocks. Depending on the method used for isolation of lignin from cellulose and hemicellulose, several types of technical lignin are available such as Kraft lignin, Sulphonate lignin (Lignosulfonate), Soda lignin and Organosolv lignin. Despite being a natural aromatic compound, lignin is mainly treated as a low value by-product, and is burned for the energy supply of pulp and paper industries. By extraction of higher value products from lignin, a renewable source of valuable chemicals would be available and the economic viabilities of the relevant industries will be promoted. Most of the recent publications have targeted one type of lignin such as Kraft lignin 1. However, it is desirable to introduce a method suitable for conversion of the range of available technical lignins. In this work, catalytic conversion of different types of lignin using an alumina supported NiMo catalyst (provided by Haldor Topsøe A/S) is conducted in ethanol at 310 °C with initial hydrogen pressure of 25 barg. The reaction time was set to 3 hours. Proton-Lignosulfonate (H-LS, provided by Borregaard A/S in form of Sodium-Lignosulfonate), Kraft lignin, Protobind 1000 and Organosolv lignin are among the selected lignin types. Non-catalytic conversion of each type of lignin was also performed at similar reaction conditions for comparison. The catalyst: lignin: solvent ratio of 1 g: 10 g: 100 ml was selected. The NiMo catalyst is a sulfur tolerant catalyst, which is originally present in the oxide form. The NiMo catalyst was presulfided before use to form NiMoS2. Presulfidation was conducted overnight by in-situ decomposition of 10 ml dimethyl disulfide and
formation of H2S.

After each standard test, the solid and liquid reaction products were separated by vacuum filtration. Furthermore, the light and heavy liquid products were separated by rotary evaporation at 35 °C and 5 mbar. While the light fraction was rich in ethanol, the remaining fraction was heavy oil, attributed as 'bio-oil'. GC-MS-FID analysis was used for identification and quantification of the bio-oil and ethanol rich light fraction. The molecular weight of the oil fraction was determined by size exclusion chromatography (SEC). Elemental analysis (Eurovector EuroEA3000) was conducted for measuring the organic C, H, S, N and O contents of the oil and solid fractions. The gas phase in the autoclave was analyzed using a gas chromatograph.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS, Borregaard
Authors: Ghafarnejad Parto, S. (Intern), Christensen, J. M. (Intern), Pedersen, L. S. (Ekstern), Taarning, E. (Ekstern), Tjosås, F. (Ekstern), Jensen, A. D. (Intern)
Number of pages: 2
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Event: Abstract from 13th European Congress on Catalysis (EUROPACAT 2017), Florence, Italy.
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Stress growth and relaxation of dendritically branched macromolecules in shear and uniaxial extension

We present unique nonlinear rheological data of well-defined symmetric Cayley-tree poly(methyl methacrylates) in shear and uniaxial extension. Earlier work has shown that their linear viscoelasticity is governed by the hierarchical relaxation of different generations, whereas the segments between branch points are responsible for their substantial strain hardening as compared to linear homopolymers of the same total molar mass at the same value of imposed stretch rate. Here, we extend that work in order to obtain further experimental evidence that will help understanding the molecular origin of the remarkable properties of these highly branched macromolecules. In particular, we address three questions pertinent to the specific molecular structure: (i) is steady state attainable during uniaxial extension? (ii) what is the respective transient response in simple shear? and (iii) how does stress relax upon cessation of extension or shear? To accomplish our goal we utilize state-of-the-art instrumentation, i.e., filament stretching rheometry (FSR) and cone-partitioned plate (CPP) shear rheometry for polymers with 3 and 4 generations, and complement it with state-of-the-art modeling predictions using the Branch-on-Branch (BoB) algorithm. The data indicates that the extensional viscosity reaches a steady state value, whose dependence on extension rate is identical to that of entangled linear and other branched polymer melts. Nonlinear shear is characterized by transient stress overshoots and the validity of the Cox-Merz rule. Remarkably, nonlinear stress relaxation is much broader and slower in extension compared to shear. It is also slower at higher generation, and rate-independent for rates below the Rouse rate of the outer segment. For extension, the relaxation time is longer than that of the linear stress relaxation, suggesting a strong 'elastic memory' of the material. These results are 2 described by BoB semi-quantitatively, both in linear and nonlinear shear and extensional regimes. Given the fact that the segments between branch points are less than 3 entanglements long, this is a very promising outcome that gives confidence in using BoB for understanding the key features. Moreover, the response of the segments between generations controls the rheology of the Cayley trees. Their substantial stretching in uniaxial extension appears responsible for strain hardening, whereas coupling of stretches of different parts of the polymer appears to be the origin of the slower subsequent relaxation of extensional stress. Concerning the latter effect, for which predictions are not available, it is hoped that the present experimental findings and proposed framework of analysis will motivate further developments in the direction of molecular constitutive models for branched and hyperbranched polymers.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, University of Crete, University of Leeds
Authors: Huang, Q. (Intern), Costanzo, S. (Ekstern), Das, C. (Ekstern), Vlassopoulos, D. (Ekstern)
Pages: 35-47
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Rheology
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ISSN (Print): 0148-6055
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 1.414 SNIP 1.553
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.413 SNIP 1.573 CiteScore 2.67
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.692 SNIP 1.584 CiteScore 3.29
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.297 SNIP 1.583 CiteScore 2.96
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.347 SNIP 1.62 CiteScore 2.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.974 SNIP 1.824 CiteScore 3.34
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.821 SNIP 1.504
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.762 SNIP 1.526
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.909 SNIP 2.504
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Scopus rating (2007): SJR 1.762 SNIP 1.78
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Web of Science (2006): Indexed yes
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Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.704 SNIP 1.785
Scopus rating (2003): SJR 1.793 SNIP 1.745
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.856 SNIP 1.994
Web of Science (2002): Indexed yes
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Web of Science (2001): Indexed yes
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Original language: English

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Structural Characterization and Enzymatic Modification of Soybean Polysaccharides

The work in this thesis explores the structure of soybean polysaccharides, and examines approaches for the chemical and enzymatic degradation and solubilization of this material. Soybean polysaccharides are produced in large quantities globally as a by-product of various soy production processes. The work presented in this text focuses on the insoluble cell wall polysaccharides produced during the manu-facture of soy protein isolate. Soybean polysaccharides are water insoluble and feature an approximate carbohydrate composition (by weight) of 35% qa-lactose, 20% glucose, 20% arabinoose, 10% galacturonic acid, 8% xylose, 3% rhamnose, and 3% fucose. Currently, the majority of this material is disposed of as waste, increasing production costs. Opportunities exist for the develop-ment of novel functional ingredients from this abundant and underutilized ma-terial; however, efforts in this area are currently limited by the material’s insol-ubility. A central hypothesis of this work was that by obtaining a more complete understanding of the structure of this material, chemical and enzymatic ap-proaches could be developed to modify the polysaccharides, creating soluble polysaccharide fractions that could provide improved functionality in industrial applications.

To address this hypothesis, structural information was obtained through HPAEC compositional analysis and GC-MS linkage analysis. This work was conducted on the whole soybean polysaccharide fraction, instead of only chemically extracted portions of this material like those analyzed in previous studies. Using this linkage data, the polysaccharide classes in soybean were quantified for the first time, with the results (by weight) identifying the primary constituents as: type I arabino-galactan (27.8%), cellulose (23.5%), (gluco-rono)arabinoxylan (14.4%), arabinan (8.1%), rhamnogalacturonan I/II (6.2%), xyloglucan (2.7%), type II arabinogalactan (2.0%), and homogalacturonan (1.6%). Using this compositional data, a novel chemical solubilization process was developed utilizing hydrogen peroxide at elevated temperatures. This treatment resulted in the release of more than 70% of the original insoluble material as high molar mass, water-soluble polysaccharides. This solubilized fraction is significantly enriched in the non-cellulosic polysaccharides of soy-bean such as arabinogalactan, homogalacturonan, rhamnogalacturonan, arabinan, xyloglucan, and (gluco-rono)arabinoxylan. These results demonstrate that it is possible to solubilize significant portions of the soybean poly-saccharide using a one-step chemical treatment, which opens new possibilities for the expanded utilization of this material going forward.

The results from this work also highlight the recalcitrance of soybean cellulose and the significant role that this polysaccharide class plays in the overall in-solubility of the material. In an effort to address this, lytic polysaccharide monoxygenases (LPMOs) were evaluated for their ability to oxidatively de-grade soybean cellulose. The initial investigations utilized TrCel61A, an AA9 LPMO from Trichoderma reesei. This enzyme showed no oxidative activity on native soybean polysaccharides; however, significant oxidative degradation was observed on NaOH pretreated soybean polysaccharides. The oxidation products were evaluated using HPAEC and MS, with the results showing oxida-tion at both the C1 and C4 positions of cellulose. In addition, a synergistic effect between TrCel61A and a GH5 endo-β-1,4-glucanase was discovered, boosting the glucose release from NaOH pretreated soybean polysaccharides.

Building upon these observations, twenty-three additional LPMOs from seven fungal sources were evaluated (using TrCel61A as a benchmark), with none showing oxidative activity on native soybean polysaccharides. However, NaOH pretreatment of the raw material was shown to improve the enzymatic accessibility of the soybean cellulose through the removal of non-cellulosic polysaccharides. Following this pretreatment, seven LPMOs (including TrCel61A) showed activity on the pretreated soybean polysaccharides. These seven enzymes were subsequently evaluated for their ability to increase the glucose release from this material through hydrolytic boosting of endo-β-1,4-glucanase and beta-glucosidase activities. Significant boosting effects were observed for TrCel61A and one of the newly evaluated LPMOs (Aspte6), re-sulting in the release of over 36% substrate glucose when compared to only 20% in the absence of the LPMO. Evaluation of the oxidation products from these LPMO treatments with HPAEC and MS showed similar C4 oxidation patterns for all soybean polysaccharide-active LPMOs. In addition, the vast majority of soybean polysaccharide-active LPMOs were also found to have oxidative activity on microcrystalline cellulose. These results demonstrate the ability of enzymatic treatments to solubilize and modify soybean polysaccharides. They also suggest new opportunities to improve upon the enzymatic digestion of this substrate in the future.

Overall, the research conducted in this project has demonstrated the utility of structure-based modification approaches and suggests that the insolubility of soybean polysaccharides is primarily conferred by the cellulosic components. In addi-tion, the results obtained suggest several new opportunities for direct chemical or enzymatic solubilization and degradation of insoluble soybean polysaccharides, paving the way for the improved utilization of this material in the future.
Structural refinement and property optimization in an Fe-23Cr-8.5Ni duplex stainless steel
An Fe-23Cr-8.5Ni duplex stainless steel was used to prepare samples with different volume-fraction-weighted grain sizes (d(α+γ)), ranging from the nano-scale to the micrometer-scale by cold rolling and subsequent annealing. The cold rolled sample with d(α+γ) of 72 nm showed a high yield strength of about 1.3 GPa but only a small tensile elongation. An abrupt increase of ductility was observed as d(α+γ) increased to 375 nm, resulting in a good combination of yield strength of 738 MPa and tensile elongation of 29%. Further increase of d(α+γ) up to the micrometer-scale results in continued decreases in yield strength but with only a limited improvement in the ductility.
comprehensive characterization.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS, Aarhus University, Karlsruhe Institute of Technology KIT

Authors: Raun, K. V. (Intern), Schumann, M. (Intern), Høj, M. (Intern), Thorhauge, M. (Ekstern), Beato, P. (Ekstern), Damsgaard, C. D. (Intern), Chevallier, J. (Forskerdatabase), Nielsen, K. (Intern), Grundwaldt, J. (Ekstern), Jensen, A. D. (Intern)

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**Studies of Deactivation of Methanol to Formaldehyde Selective Oxidation Catalyst**

Formaldehyde (CH₂O) may be synthesized industrially by selective oxidation of methanol over an iron-molybdate (Fe-Mo) oxide catalyst according to: CH₃OH + ½O₂ → CH₂O + H₂O. The reaction is normally carried out in a multitubular reactor with excess of air at 250-400 °C (yield = 90-95 %), known as the Formox process [1]. The average lifetime of the industrial catalyst is only 1–2 years depending on the operating conditions. The catalyst consists of a bulk phase of Fe₂(MoO₄)₃ and a surface layer phase of MoO₃. The MoO₃ surface is selective towards formaldehyde while the iron in the sublayer increases the activity of the catalyst [2]. Pure MoO₃ in itself has low activity. Literature from the last decades agrees that the major reason for the deactivation is loss of molybdenum from the catalyst. Molybdenum forms volatile species with methanol, which can leave behind Mo poor zones. The catalyst is usually prepared with excess MoO₃ (Mo/Fe > 1.5) to counter the loss of Mo. This work focuses on understanding the structural changes occurring in the catalyst and its behavior during deactivation via prolonged activity testing and spectroscopic investigations.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS, Aarhus University, Karlsruhe Institute of Technology KIT

Authors: Raun, K. V. (Intern), Schumann, M. (Ekstern), Høj, M. (Intern), Dalslet, B. T. (Ekstern), Beato, P. (Ekstern), Damsgaard, C. D. (Intern), Chevallier, J. (Ekstern), Grundwaldt, J. (Ekstern), Jensen, A. D. (Intern)

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**Superstructure-based optimization tool for plant design and retrofitting**

Many wastewater treatment processes and technologies have been developed since the beginning of the 20th century to meet increasingly stringent performance demands. Still the wastewater industry has been facing many new challenges such as increasing energy costs, presence of trace organics which has become more critically investigated, depletion of the resources, water conservation as well as more stringent regulations (Reardon et al. 2013).

**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre

Authors: Bozkurt, H. (Intern), Gemaey, K. V. (Intern), Sin, G. (Intern)

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Supervisory Model Predictive Control of the Heat Integrated Distillation Column

This paper benchmarks a centralized control system based on model predictive control for the operation of the heat integrated distillation column (HIDiC) against a fully decentralized control system using the most complete column model currently available in the literature. The centralized control system outperforms the decentralized system, because it handles the interactions in the HIDiC process better. The integral absolute error (IAE) is reduced by a factor of 2 and a factor of 4 for control of the top and bottoms compositions, respectively.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre
Authors: Meyer, K. (Intern), Bisgaard, T. (Intern), Huusom, J. K. (Intern), Abildskov, J. (Ekstern)
Pages: 7375-7380
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Scopus rating (2008): SJR 0.125 SNIP 0.105
Scopus rating (2007): SJR 0.126 SNIP 0.065
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Supply Chain Optimization of Integrated Glycerol Biorefinery: GlyThink Model Development and Application

To further advance the development and implementation of glycerol-based biorefinery concepts, it is critical to analyze the glycerol conversion into high value-added products in a holistic manner, considering both production as well as the logistics aspects related to the supply chain structure. To address the optimal design and planning of the glycerol-based biorefinery supply chain, in this work, we propose a multiperiod, multistage, and multiproduct Mixed Integer Linear Programming optimization model, called GlyThink, based upon the maximization of the net present value (NPV). The proposed model is able to identify operational decisions, including locations, capacity levels, technologies, and product
portfolio, as well as strategic decisions such as inventory levels, production amounts, and transportation to the final markets. Several technologies are considered for the glycerol valorization to high value-added products. Existing countries with major production and consumption of biodiesel in Europe are considered as candidates for the facility sites and demand markets, and their spatial distribution is also carefully studied. The results showed that (i) the optimal solution that provides the best NPV is obtained by establishing a multiproduct supply chain for the glycerol-based integrated biorefinery, built upon four plant site locations (Germany, France, The Netherlands, and Italy); (ii) if a single-plant alternative is to be selected, Germany stands out as potentially the best location for the integrated biorefinery; (iii) government incentives might play a decisive role in the growth of a glycerol-based economy showing improved economic feasibility; and, last, (iv) the optimal product portfolio suggested is based on the production of succinic acid and lactic acid, followed by epichlorohydrin and poly-3-hydroxybutyrate (PHB).

**General information**

**State:** Published  
**Organisations:** Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidade de Lisboa  
**Authors:** Loureiro da Costa Lira Gargalo, C. (Intern), Carvalho, A. (Ekstern), Gernaey, K. (Intern), Sin, G. (Intern)  
**Pages:** 6711-6727  
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ISI indexed (2012): Indexed yes  
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BFI (2008): BFI-level 2  
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Scopus rating (2008): SJR 1.142 SNIP 1.267
Surface-Initiated Atom Transfer Radical Polymerization from Electrospun Mats: An Alternative to Nafion

Proton exchange membranes for fuel cell applications are synthesized by surface-initiated (SI) atom transfer radical polymerization (ATRP). Poly(vinylidene fluoride-co-chlorotrifluoroethylene) is electrospun into 50 μm thick mat, which is then employed as multifunctional initiator for copper-mediated SI ATRP of 4-styrene sulfonic acid sodium salt. Fine-tuning of the ATRP conditions allows adjustment of the membrane's ion exchange capacity by varying the loading of the grafted ionomer. Structure and composition of the membranes are investigated by spectroscopic means and thermogravimetric analysis, respectively. The membrane morphology is probed by scanning electron microscopy. A membrane with proton conductivity as high as 100 mS cm\(^{-1}\) is obtained. Long-term durability study in direct methanol fuel cells is conducted for over 1500 h demonstrating the viability of this novel facile approach.
Surface properties correlate to the digestibility of hydrothermally pretreated lignocellulosic Poaceae biomass feedstocks

Background: Understanding factors that govern lignocellulosic biomass recalcitrance is a prerequisite for designing efficient 2nd generation biorefining processes. However, the reasons and mechanisms responsible for quantitative differences in enzymatic digestibility of various biomass feedstocks in response to hydrothermal pretreatment at different severities are still not sufficiently understood.

Results: Potentially important lignocellulosic feedstocks for biorefining, corn stover (Zea mays subsp. mays L.), stalks of Miscanthus × giganteus, and wheat straw (Triticum aestivum L.) were systematically hydrothermally pretreated; each at three different severities of 3.65, 3.83, and 3.97, respectively, and the enzymatic digestibility was assessed. Pretreated samples of Miscanthus × giganteus stalks were the least digestible among the biomass feedstocks producing ~24 to 66.6% lower glucose yields than the other feedstocks depending on pretreatment severity and enzymedosage. Bulk biomass composition analyses, 2D nuclear magnetic resonance, and comprehensive microarray polymer profiling were not able to explain the observed differences in recalcitrance among the pretreated feedstocks. However, methods characterizing physical and chemical features of the biomass surfaces, specifically contact angle measurements (wettability) and attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy (surfacebiopolymer composition) produced data correlating pretreatment severity and enzymatic digestibility, and they also revealed differences that correlated to enzymatic glucose yield responses among the three different biomass types.

Conclusion: The study revealed that to a large extent, factors related to physico-chemical surface properties, namely surface wettability as assessed by contact angle measurements and surface content of hemicellulose, lignin, and waxes assessed by ATR-FTIR rather than bulk biomass chemical composition correlated to the recalcitrance of the tested biomass types. The data provide new insight into how hydrothermal pretreatment severity affects surface properties of key Poaceae lignocellulosic biomass and may help design new approaches to overcome biomass recalcitrance.
**Sustainable chemical processing and energy-carbon dioxide management: review of challenges and opportunities**

This paper presents a brief review of the available energy sources for consumption, their effects in terms of CO2-emission and its management, and sustainable chemical processing where energy-consumption, CO2-emission, as well as economics and environmental impacts are considered. Not all available energy sources are being utilized efficiently, while, the energy source causing the largest emission of CO2 is being used in the largest amount. The CO2 management is therefore looking at "curing" the problem rather than "preventing" it. Examples highlighting the synthesis, design and analysis of sustainable chemical processing in the utilization of biomass-based energy-chemicals production, carbon-capture and utilization with zero or negative CO2-emission to produce value added chemicals as well as retrofit design of energy intensive chemical processes with significant reduction of energy consumption are presented. These examples highlight issues of energy sustainable design, energy-CO2 neutral design, energy-retrofit design, and energy-process intensification. Finally, some perspectives on the status and future directions of carbon dioxide management are given.

**General information**

State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, National Institute of Technology Warangal
Authors: Frauzem, R. (Intern), Vooradi, R. (Ekstern), Bertran, M. (Intern), Frauzem, R. (Intern), Anne, S. B. (Ekstern), Gani, R. (Intern)
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  - Web of Science (2017): Indexed yes
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  - Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
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  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 0.957 SNIP 1.668 CiteScore 2.56
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  - Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
  - ISI indexed (2012): ISI indexed yes
  - BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 0.912 SNIP 1.335 CiteScore 2.12
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 1
  - Scopus rating (2010): SJR 0.87 SNIP 1.317
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 1
  - Scopus rating (2009): SJR 0.742 SNIP 1.029
Sustainable process design with process intensification - Development and implementation of a framework for sustainable carbon dioxide capture and utilization processes

Due to environmental concerns, greenhouse gas emissions, particularly carbon dioxide, need to be reduced. There are numerous methods being discussed, one of which is carbon dioxide capture and utilization (CCU). Carbon dioxide capture and utilization removes the carbon dioxide from the offgas streams and transforms it into commercial products, for example the conversion to value-added chemicals. While CCU is promising, especially as the commercial products provide an economic incentive, the sustainability needs to be ensured. Assuring the sustainability of carbon dioxide capture and utilization processes is a challenge as the energy requirements result in indirect emissions that should not exceed the utilization. In this work, therefore, a framework for the sustainable design of carbon dioxide capture and utilization (with a focus on conversion) processes is developed and implemented.

The developed framework adopts a 3-stage approach for sustainable design, which is comprised of: (1) synthesis, (2) design, and (3) innovation. In the first stage, the optimal processing route is obtained from a network via a superstructure-based approach. This stage incorporates a structured database for the storage and retrieval of data, reaction path synthesis for the generation of reaction pathways and products, and a user interface, Super-O, which facilitates the implementation of Stage 1 of the framework. Then, the output of this stage is used as the input to the second stage, where the optimal route is rigorously designed, simulated and analyzed. Stage 2 provides detailed equipment design and stream information, which is used in the analysis to provide targets for improvement. In Stage 3, the targets are addressed by finding innovative alternatives via hybrid methods, process integration and process intensification. The end result is a more sustainable carbon dioxide capture and utilization process. The developed framework is then applied to the design of sustainable processes using carbon dioxide captured from a coal-fired power plant (as these represent almost 30% of global emissions). In the first stage, seven scenarios are considered to evaluate the influence of different parameters (such as prices and conversion) in finding the optimal processing route(s). The results show a trade-off in the reduction of carbon dioxide and the profit for the different routes. From Stage 1, four processes are considered and are designed and simulated in detail:
1. Dimethyl ether from methanol via combined reforming
2. Dimethyl ether from methanol via direct hydrogenation
3. Dimethyl carbonate via ethylene carbonate and methanol from combined reforming
4. Dimethyl carbonate via ethylene carbonate and methanol from direct hydrogenation.

Through the analysis of the processes, it can be seen that the methanol distillation and the dimethyl carbonate downstream separation contribute to large amounts of the utility consumption and therefore costs. Therefore, the reduction of the utility consumption of the methanol distillation and dimethyl carbonate downstream process are targeted for improvement. In Stage 3, the targets are addressed by introducing a hybrid distillation-membrane process and an intensified, reactive distillation dimethyl carbonate process. The result is four improved, more sustainable processes for the production of dimethyl ether and dimethyl carbonate from carbon dioxide. However, while it is possible to design carbon dioxide reducing processes, the amount of emissions that can be offset by these processes is small. Therefore, these...
carbon dioxide capture and utilization or conversion processes should be considered in conjunction with methods to improve efficiency and other alternative, sustainable processes.

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Authors: Frauzem, R. (Intern)
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Sustainable process design with process intensification - Development and implementation of a framework for sustainable carbon dioxide capture and utilization processes
Publication: Research › Ph.D. thesis – Annual report year: 2018

**Synthesis of a novel polyester building block from pentoses by tin-containing silicates**
We report here the direct formation of the new chemical product, trans-2,5-dihydroxy-3-pentenoic acid methyl ester, from pentoses using tin-containing silicates as catalysts. The product is formed under alkali-free conditions in methanol at temperatures in the range 140–180 °C. The highest yields are found using Sn-Beta as the catalyst. Under optimised conditions, a yield of 33% is achieved. Purified trans-2,5-dihydroxy-3-pentenoic acid methyl ester was used for copolymerisation studies with ethyl 6-hydroxyhexanoate using Candida antarctica Lipase B as the catalyst. The copolymerisation yields a product containing functional groups originating from trans-2,5-dihydroxy-3-pentenoic acid methyl ester in the polyester backbone. The reactivity of the incorporated olefin and hydroxyl moieties was investigated using trifluoroacetic anhydride and thiol-ene chemistry, thus illustrating the potential for functionalising the new co-polymers.

**General information**
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Organisations: Department of Chemistry, Organic Chemistry, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Haldor Topsoe AS
Authors: Elliot, S. G. (Intern), Andersen, C. (Intern), Tolborg, S. (Intern), Meier, S. (Intern), Sadaba, I. (Ekstern), Daugaard, A. E. (Intern), Taarning, E. (Ekstern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Targeted pre-treatment of hemp bast fibres for optimal performance in biocomposite materials: A review

Global interest in the use of plant fibres in natural fibre reinforced composites (NFCs) is growing rapidly. The increased interest is primarily due to the advantageous properties of natural fibres including biodegradability, low cost, low density and high stiffness and strength to weight ratio. In order to achieve strong NFCs, well separated and cellulose-rich fibres are required. Hemp is taking a center stage in this regard as a source of suitable natural plant cellulose fibres because natural hemp bast fibres are long and inherently possess high strength. Classical field and water retting methods have been used for centuries for removal of non-cellulosic components from fibrous plant stems including from hemp, but carries a risk of reducing the mechanical properties of the fibres via damaging the cellulose. For NFCs new targeted fibre pre-treatment methods are needed to selectively and effectively remove non-cellulosic components from the plant fibres to produce cellulose rich fibres without introducing any damage to the fibres. A key feature for successful use of natural fibres such as hemp fibres in composite materials is optimal interfacial contact between the fibres and the hydrophobic composite matrix material. Targeted modification of natural fibres for NFCs must also be targeted to optimize the fibre surface properties. Consequently, improved interfacial bonding between fibres and hydrophobic polymers, reduced moisture uptake, increased microbial degradation resistance, and prolonged durability of NFCs can be achieved. This review, using hemp bast fibres as an example, critically and comprehensively assesses the targeted pretreatment technologies and data available for producing well separated cellulose bast fibres having optimal chemical and physical properties for maximizing the mechanical performance and durability of NFCs.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, University of Plymouth
Authors: Liu, M. (Intern), Thygesen, A. (Intern), Summerscales, J. (Ekstern), Meyer, A. S. (Intern)
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Scopus rating (2016): CiteScore 3.78 SJR 1.059 SNIP 1.657
Web of Science (2016): Indexed yes
Tar Removal from Biomass Producer Gas by Using Biochar

The biomass-derived char (biochar) produced in the gasifier as a residue, is a potential solution for removing tars from producer gas. This work investigates the interaction between tar compounds and biochar. Residual biochar from a TwoStage gasifier was tested as bed material in a laboratory setup. Phenol and naphthalene were chosen as model tars, and entrained in a nitrogen flow. The gaseous stream was sampled before and after the biochar bed to evaluate the extent of conversion. The biochar bed (30g) was tested at 250°C, 500°C and 600°C, with for 3 consecutive hours. The compounds concentration in the gas phase was quantified by stable isotope dilution analysis, using Gas Chromatography-Mass Spectrometry (GC-MS). Results showed a significant effect of biochar on the removal of phenol, at all temperatures. Naphthalene was removed less efficiently at higher temperature, and this trend was even more visible with a smaller char bed (17g). The characterization of the residual biochar from the TwoStage gasifier showed high carbon content and a
specific surface area comparable with active carbon. Scanning Electron Microscopy revealed that the wood structure is largely maintained in the biochar particles, and the main inorganic components are calcium, potassium and silicon in form of oxides.

**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre

Authors: Ravenni, G. (Intern), Henriksen, U. B. (Intern), Ahrenfeldt, J. (Intern), Sárossy, Z. (Intern)

Pages: 473-477

Publication date: 2017

**Host publication Information**

Title of host publication: Proceedings of the 25th European Biomass Conference and Exhibition

Publisher: ETA-Florence Renewable Energies


Main Research Area: Technical/natural sciences

Conference: 25th European Biomass Conference and Exhibition, Stockholm, Sweden, 12/06/2017 - 12/06/2017

Gas cleaning, Gasification, Tar removal, Biochar

**Techno-economic analysis of resource recovery technologies for wastewater treatment plants**

The high nutrient content of domestic wastewater can be efficiently recovered through specific technologies included in dedicated wastewater treatment plants (WWTPs). Nevertheless, the operational costs linked to the implementation of these technologies can make them economically unfeasible. It is therefore important to evaluate the best way to upgrade an already existing WWTP from an economic point of view. In the present work, this is virtually done by using a simulation model, namely the Benchmark Simulation Model no2 (BSM2), as base case study. The BSM2 is extended by including the following resource-recovery treatment units: (a) a chemical precipitation process, for recovery of iron phosphate fertilizer; (b) the Exelys technology, for increased biogas production; and, (c) the Phosnix technology, for recovery of struvite fertilizer. Seven upgrade strategies/flowsheets employing different combinations of the recovery technologies are generated and evaluated. The evaluation results have shown that the most economically beneficial strategy to upgrade the WWTP is to employ a Phosnix reactor in the side-stream to recover phosphorus from the bottom of the dewatering treatment unit. All other upgrading combinations involving chemical precipitation and Exelys technologies were not found economical for the given plant. Sensitivity analyses on the economic evaluation criteria have demonstrated that the results obtained are robust against uncertainties in influent wastewater characteristics and technical (e.g. recovery yield) performance parameters.

**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidade de Lisboa

Authors: Boiocchi, R. (Intern), Matafome, B. (Ekstern), Loureiro da Costa Lira Gargalo, C. (Intern), Carvalho, A. (Ekstern), Sin, G. (Intern)

Pages: 1945-1950

Publication date: 2017

**Host publication Information**

Title of host publication: Proceedings of the 27th European Symposium on Computer Aided Process Engineering (ESCAPE 27)

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Editors: Espuña, A., Graells, M., Puigjaner, L.

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DOIs: 10.1016/B978-0-444-63965-3.50326-3

Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

**The Chemical Product Simulator - ProCAPD**

In this paper, a chemical product design simulator called ProCAPD is presented. ProCAPD works in the same way as a chemical process simulator, that is, it helps to verify product design decisions and generates information that can be used
to make design decisions. Like the contents of the process simulator, the product simulator needs a database of chemicals and properties, a library of models, numerical routines to solve mathematical problems as well as various calculation options. Also, like the process simulator, the product simulator comes with a user-interface to describe the problems and to obtain the simulation results. In order to make the chemical product simulator versatile and applicable for a wide range of problems, it includes a suite of databases (chemicals, solvents, active ingredients, aroma, color-agents and many more); a library of models (properties, product performance, etc.); calculation tools (product attributes, blend compositions, environmental impact, etc.); design templates (single molecules, blends, formulations, emulsions, devices); and, design-simulation-analysis functions. All these capabilities are based on the prototype tool developed by Kalakul et al. (2017). This paper highlights the software architecture, the implemented computer aided methods-tools, whose scope-significance are illustrated through new chemical product design-evaluation applications.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Auburn University
Authors: Kalakul, S. (Ekstern), Eden, M. R. (Ekstern), Gani, R. (Intern)
Pages: 979-984
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Publisher: Elsevier
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Main Research Area: Technical/natural sciences
Conference: 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 01/10/2017 - 01/10/2017
Chemical product design, Product-process simulator, Blended products, Formulations, Single molecular products
DOI: 10.1016/B978-0-444-63965-3.50165-3
Source: FindIt
Source-ID: 2394577709
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

The effect of design and scale on the mixing and mass transfer in U-loop bioreactors
A system capable of handling a large volumetric gas fraction while providing a high gas to liquid mass transfer is a necessity if the methanotrophic bacterium Methylococcus capsulatus is to be used in single cell protein (SCP) production. Previous studies have proven that a U-loop fermenter, a novel vertical forced flow loop reactor where gas and liquid are driven through a series of static mixers in a U-shaped pipe, is quite capable of coping with these challenges in pilot scale. The critical question remains; what happens when the scale undergoes a more than 10 fold increase and the geometry is altered?

In this study we have investigated the mixing time and mass transfer capabilities of U-loop reactors of different geometries (high vs. diameter ratio) in pilot (0.15m3) and semi-industrial scales (2.2m3). A new expression for the mechanical power input into the system is also proposed, which indicates that an even more favorable relationship between power input and mass transfer rate (compared to previous literature) applies to U-loop fermenters.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, CHEC Research Centre, PILOT PLANT, Unibio A/S
Authors: Petersen, L. A. H. (Intern), Villadsen, J. (Intern), Jørgensen, S. B. (Intern), Christensen, I. (Ekstern), Eliasson Lantz, A. (Intern), Gernaey, K. V. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from Recent Advances in Fermentation Technology (RAFT 2017), Florida, United States.
Main Research Area: Technical/natural sciences
Electronic versions: abstract.pdf
Source: PublicationPreSubmission
Source-ID: 139748117
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017
The Effect of Pt Particle Size on the Oxidation of CO, C\textsubscript{3}H\textsubscript{6}, and NO Over Pt/Al\textsubscript{2}O\textsubscript{3} for Diesel Exhaust Aftertreatment

Platinum-based oxidation catalysts applied for diesel exhaust aftertreatment constitute a significant part of system costs. Effective utilization of platinum is therefore relevant to reduce costs while retaining performance. To this end, the influence of Pt particle size on catalytic activity for CO, hydrocarbon, and NO oxidation was studied. 1 wt% Pt/Al\textsubscript{2}O\textsubscript{3} catalysts were prepared by wet impregnation, drying, and different calcination and thermal treatments, yielding Pt particles with diameters between 1.3 and 18.7 nm, as determined by CO pulse titration and transmission electron microscopy. Activity measurements for CO, C\textsubscript{3}H\textsubscript{6}, and NO oxidation showed an optimal Pt particle size with respect to the mass based activity between 2 and 4 nm for all three reactions. From measured turnover frequencies and site statistics of Pt particles, the reactions appear to be mainly catalyzed by terrace atoms, which are most abundant between 2 and 4 nm. The decrease in catalytic activity for large Pt particles is therefore due to the diminishing Pt surface area, while the decrease in activity for small particles is due to the lack of terrace atoms required for CO, HC, and NO oxidation.
The effects of concentration and heating-cooling rate on rheological properties of Plantago lanceolata seed mucilage

In this study, the effect of concentration (0.5, 1, 1.5 and 2%) and heating-cooling rate (1, 5 and 10 °C min−1) on the rheological properties of Plantago lanceolata seed mucilage (PLSM) solutions were investigated. It was observed that the gum dispersions exhibited viscoelastic properties under the given conditions. Mechanical spectra of PLSM were classified as weak gels based on the frequency sweep, complex viscosity (η*) and tan δ results. All variables had significant impacts on the rheological parameters. Chemical and monosaccharide compositions were also determined to provide more structural information. The results revealed that PLSM had high total sugar content (87.35%), and it is likely an arabinoxylomannan-type polysaccharide.

General information
State: Accepted/In press
Organisations: National Food Institute, Research Group for Nano-Bio Science, Research Group for Food Production Engineering, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Ferdowsi University of Mashhad
Authors: Hesarinejad, M. A. (Ekstern), Sami Jokandan, M. (Intern), Mohammadifar, M. A. (Intern), Koocheki, A. (Ekstern), Razavi, S. M. A. (Ekstern), Ale, M. T. (Intern), Attar, F. R. (Ekstern)
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Biological Macromolecules
ISSN (Print): 0141-8130
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.84 SJR 0.872 SNIP 1.288
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.815 SNIP 1.316 CiteScore 3.38
Web of Science (2015): Indexed yes
The mechanism of fracture for entangled polymer liquids in extensional flow

In uniaxial extensional flow of entangled polymer liquids, different rupture modes may happen, including necking and fracture. Malkin and Petrie [1] proposed a "master curve" dividing the flow behavior into four zones based on the stretch rate: (I) Flow zone; (II) Transition zone; (III) Rubbery zone; and (IV) Glass-like zone. The master curve shows that steady extensional flow can only be reached in Zone I where the stretch rate is very slow, while rupture happens in Zones II-IV with faster stretch rate. Furthermore, Wang et al. [2-4] reported experimental data that matches the master curve and suggested the mechanism of rupture in Zone III and IV is disentanglement and chain scission, respectively. In this work we measure two groups of entangled polystyrene solutions. In one group the samples have the same entanglement molecular weight (Me) but different number of entanglements (Z), and in the other group the samples have the same Z but different Me. We show that uncontrolled filament stretching, steady extensional flow can be reached in Zones I-III, while fracture happens in Zone IV. The critical strain at fracture decreases with increasing stretch rate, which is in agreement with the master curve in Zone IV. However, with faster rate, a constant critical strain is observed, which is not shown in the original master curve. The value of the constant critical strain seems to be related to the maximum stretch ratio of the polymer chain (determined by Me), but not influenced by Z. The results are also compared with the critical strain of chemically crosslinked polymer networks.
The mechanism of fracture for entangled polymer liquids in extensional flow

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Huang, Q. (Intern), Yu, L. (Intern), Skov, A. L. (Intern), Hassager, O. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from The Annual European Rheology Conference (AERC2017), Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
AERC2017_QianHuang.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Thermodynamic Analysis of Chalk–Brine–Oil Interactions
The surface complexity models (SCMs) are used successfully for describing the thermodynamic equilibrium between the pure calcite surface (carbonate and calcium sites) and brine solutions. In this work, we show that the model parameters that are reported for the calcite–brine system are not applicable to the natural carbonates. We adjust the SCM reaction equilibrium constants by fitting the model to the ζ potential data that are reported for the pulverized Stevns Klint chalk. Then, we use the model, implemented in the PhreeqcRM geochemistry package coupled with a finite volume solver, to predict the breakthrough composition of different ions in the chromatographic experiments on the intact Stevns Klint chalk cores. Again, the model falls short in predicting the reactive transport of brine in a natural carbonate, implying that ζ potential data is not enough for optimizing the SCM model parameters for the reactive transport applications. We propose an optimization procedure that fits the coupled SCM–transport model parameters to the chromatographic (single-phase core flooding) data. The ζ potential measurements are implemented in the optimization scheme as nonlinear constraints. We then use the optimized model to study the thermodynamic equilibrium between the oil and chalk surfaces in the presence of different brine compositions, including the dissolution and precipitation of minerals. We represent the chalk–oil interactions by acid–base equilibrium reactions between the calcium and carbonate sites on the chalk surface and carboxylic acids and amine bases on the oil surface, respectively. Comparing the model results to a data set of the spontaneous imbibition experiments for chalk shows that the remaining oil saturation in the imbibition experiments is correlated with the number of bonds between the amine and carboxylate groups on the oil surface and the carbonate and protonated calcium on the chalk surface.

General information
State: Published
Organisations: Centre for oil and gas – DTU, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Authors: Eftekhari, A. A. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern), Nick, H. M. (Intern)
Pages: 11773–11782
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
Journal: Energy and Fuels
Volume: 31
Issue number: 11
ISSN (Print): 0887-0624
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Thermodynamic modelling of acid gas removal from natural gas using the Extended UNIQUAC model

Thermodynamics of natural gas sweetening process needs to be known for proper design of natural gas treating plants. Absorption with aqueous N-Methyldiethanolamine is currently the most commonly used process for removal of acid gas (CO₂ and H₂S) impurities from natural gas. Model parameters for the Extended UNIQUAC model have already been determined by the same authors to calculate single acid gas solubility in aqueous MDEA. In this study, the model is further extended to estimate solubility of CO₂ and H₂S and their mixture in aqueous MDEA at high pressures with methane as a makeup gas.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering
Authors: Sadegh, N. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
The Systematic Screening Methodology for Surfactant Flooding Chemicals in Enhanced Oil Recovery

The product design framework for systematic screening & selection of surfactants consists of four main steps: problem definition, target properties specification, data collection & model development, and screening-selection. The Hydrophilic-Lipophilic Deviation (HLD) value has been identified as the main target property because it is related to the microemulsion type of a surfactant-oil-water system. That is, when the HLD value is zero, the middle-phase microemulsion, which has the lowest interfacial tension of oil and water, is formed. The model for HLD estimation needs a parameter Cc, which is predicted by a group-contribution technique. The developed group-contribution model for anionic surfactants gives relative error equal to 3.5, while the model for non-ionic surfactants does not give very good relative error, mainly because of small values of Cc and not enough data. Nevertheless, the model for non-ionic surfactants is found to be qualitatively correct and so it can be used for surfactant screening-selection. Other properties like melting point, cloud-point, etc., are also used for the screening-selection step. Application of the model-based method is highlighted through two case studies, where the results have been verified experimentally.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Chulalongkorn University
Authors: Cholpraves, C. (Ekstern), Rattanaudom, P. (Ekstern), Suriyapraphadilok, U. (Ekstern), Charoensaeng, A. (Ekstern), Gani, R. (Intern)
Pages: 991-996
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the 27th European Symposium on Computer Aided Process Engineering – ESCAPE 27
Volume: 40
Publisher: Elsevier
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Series: Computer - Aided Chemical Engineering
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 01/10/2017 - 01/10/2017
Enhanced Oil Recovery, Microemulsion, Surfactant, Group-contribution, Hydrophilic-Lipophilic Deviation
DOIs: 10.1016/B978-0-444-63965-3.50167-7
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

The transition between undiluted and oligomer-diluted states of nearly monodisperse polystyrenes in extensional flow
We have measured the startup and steady extensional viscosity of two narrow molar mass distributed (NMMD) polystyrenes, a 910 kg/mole and a 545 kg/mole, diluted in a NMMD 4.29 kg/mole styrene oligomer, with a wide concentration range from 90 down to 17%. The constant interchain pressure model, proposed by Rasmussen and Huang (Rheol Acta 53(3):199–208 (2014a)), predicts the extensional viscosity well for the dilutions with lower concentrations. However, for the 70 and 90% 545 kg/mole samples which represent the transition between the diluted and undiluted states, the model predictions are less satisfactory. Another concept based on interchain pressure, proposed by Wagner (Rheol Acta 53(10):765–777 (2014)), also shows agreement with the measured data.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Mechanical Engineering, Manufacturing Engineering
Toward a sustainable biorefinery using high-gravity technology

The realization of process solutions for a sustainable bioeconomy depends on the efficient processing of biomass. High-gravity technology is one important alternative to realizing such solutions. The aims of this work were to expand the knowledge-base on lignocellulosic bioconversion processes at high solids content, to advance the current technologies for production of second-generation liquid biofuels, to evaluate the environmental impact of the proposed process by using life cycle assessment (LCA), and to develop and present a technically, economically, and environmentally sound process at high gravity, i.e., a process operating at the highest possible concentrations of raw material. The results and opinions presented here are the result of a Nordic collaborative study within the framework of the HG Biofuels project. Processes with bioethanol or biobutanol as target products were studied using wheat straw and spruce wood at a dry matter content of 30% (w/w) as model substrates. The LCA performed revealed the environmental impact of each of the process steps, highlighting the importance of the enzyme dose used for the hydrolysis of the plant biomass, as well as the importance of the fermentation yield. (c) 2016 The Authors. Biofuels, Bioproducts and Biorefining published by Society of Chemical Industry and John Wiley & Sons, Ltd.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Chalmers University of Technology, SEKAB, Statoil ASA, University of Copenhagen
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Main Research Area: Technical/natural sciences

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Volume: 11
Issue number: 1
ISSN (Print): 1932-104X
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.58 SJR 1.114 SNIP 1.291
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.643 SNIP 1.451 CiteScore 3.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.74 SNIP 1.704 CiteScore 3.92
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.821 SNIP 1.867 CiteScore 4.49
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.487 SNIP 1.656 CiteScore 3.56
ISI indexed (2012): ISI indexed yes
In this study, Bacillus licheniformis 421 was used as a model organism to understand the effects of microbial cell growth and metabolite production under anaerobic conditions in relation to microbial enhanced oil recovery. The bacterium was able to grow anaerobically on different carbon compounds, where n-alkanes were preferred over molasses as carbon source. The bacterium grew slowly when n-alkanes were used as carbon source, however, formation of emulsions and reduction of interfacial tension (IFT) were still observed. The bacterial cells were mainly present at the interface of the synthetic seawater medium and the n-alkanes. The bacterium produced lipopeptide lichenysin G which was detected both in the water and in the emulsion phase. We propose that the bacterial cells themselves or metabolites attached to the cell surface are the main players in the formation of emulsions and IFT reduction.
In-sewer transformation of drug biomarkers (excreted parent drugs and metabolites) can be influenced by the presence of biomass in suspended form as well as attached to sewer walls (biofilms). Biofilms are likely the most abundant and biologically active biomass fraction in sewers. In this study, 16 drug biomarkers were selected, including the major human metabolites of mephedrone, methadone, cocaine, heroin, codeine and tetrahydrocannabinol (THC). Transformation and sorption of these substances were assessed in targeted batch experiments using laboratory-scale biofilm reactors operated under aerobic and anaerobic conditions. A one-dimensional model was developed to simulate diffusive transport, abiotic and biotic transformation and partitioning of drug biomarkers. Model calibration to experimental results allowed estimating transformation rate constants in sewer biofilms, which were compared to those obtained using in-sewer suspended biomass. Our results suggest that sewer biofilms can enhance the transformation of most compounds.

Through scenario simulations, we demonstrated that the estimation of transformation rate constants in biofilm can be significantly biased if the boundary layer thickness is not accurately estimated. This study complements our previous investigation on the transformation and sorption of drug biomarkers in the presence of only suspended biomass in untreated sewage. A better understanding of the role of sewer biofilms—also relative to the in-sewer suspended solids—and improved prediction of associated fate processes can lead to more accurate estimation of daily drug consumption in urban areas.
areas in wastewater-based epidemiological assessments.

**General information**

State: Published
Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, Environmental Chemistry, KWR Watercycle Research Institute, University of Amsterdam
Authors: Ramin, P. (Intern), Brock, A. L. (Intern), Causanilles Llanes, A. (Ekstern), Valverde Pérez, B. (Intern), Emke, E. (Ekstern), de Voogt, P. (Ekstern), Polesel, F. (Intern), Plósz, B. G. (Intern)
Pages: 10572–10584
Publication date: 2017
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**Publication information**

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Volume: 51
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  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 2
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 2
  - Scopus rating (2016): CiteScore 6.26 SJR 2.538 SNIP 1.889
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 2
  - Scopus rating (2015): SJR 2.584 SNIP 1.828 CiteScore 5.61
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 2
  - Scopus rating (2014): SJR 2.777 SNIP 2.017 CiteScore 5.5
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 2
  - Scopus rating (2013): SJR 2.956 SNIP 2.103 CiteScore 5.52
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 2
  - Scopus rating (2012): SJR 3.146 SNIP 2.056 CiteScore 5.17
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 2
  - Scopus rating (2011): SJR 3.178 SNIP 1.953 CiteScore 5.16
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 2.964 SNIP 1.729
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 2
  - Scopus rating (2009): SJR 2.835 SNIP 1.803
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 2
  - Scopus rating (2008): SJR 2.943 SNIP 1.942
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 2.8 SNIP 1.927
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 2.541 SNIP 1.901
  - Web of Science (2006): Indexed yes
  - Scopus rating (2005): SJR 2.604 SNIP 2.014
Ultrasonication has been proposed as a promising technique for enzymatic transesterification. In contrast, excess ultrasonication causes an enzyme inactivation. This paper presents enzymatic transesterification to produce fatty acid methyl ester (FAME) from rapeseed oil using Callera Trans L™ using a an original two-compartment reactor. The reactor was composed of a mechanically stirred compartment (ST) and ultrasound irradiation compartment (US). The reaction solution was recirculated between the ST and the US. The enzyme was only exposed by ultrasonication in the US. The reactor system has the option to control the direct irradiation period of ultrasonication to soluble enzyme, regulated by the mean residence time in the US.
Uncertainty & sensitivity analysis of economic assessment of lactic acid production from crude glycerol - impact of price correlations

In this work, we investigate the impact of the expected price volatility and correlations on the overall economic assessment of lactic acid production from crude glycerol. In particular, the goals of this study are three-fold: (i) to understand how uncertainty in the inputs propagates to the model outputs; (ii) to understand the effect of the degree of pairwise correlation between input uncertainties on each other and on the outputs from the economic model (Net Present Value); and lastly, (iii) to estimate the first-order as well as independent sensitivity indices so as to identify which of the input uncertainties in the economic analysis affect the estimated NPV the most. To this end, we implemented algorithms in Matlab (R2015a) based on Monte Carlo sampling with permutation using Latin Hypercube Sampling with Iman Conover correlation control (Sin et al., 2009). The results have shown that the estimated NPVs are very sensitive to uncertainties in the inputs. In particular, not only the magnitude of the input uncertainty but also the degree and the sign of the correlation among input uncertainties matter a lot. All in all, this approach aims at providing information and powerful insights on the quality of the estimated NPV, a commonly used economic indicator, for assessing high risk and high gain biotech process investments. The results help to better assess economic feasibility under a broad range of uncertainties and ultimately minimize the risk of potential business failure commonly seen in past biorefinery developments.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidade de Lisboa
Uncertainty Analysis for the Parameterization of Glycols

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
Authors: Kruger, F. (Intern)
Event: Poster session presented at 29th European Symposium on Applied Thermodynamics, Bucharest, Romania.
Main Research Area: Technical/natural sciences
Electronic versions: ESAT_2017_Poster_v4b.pdf
Publication: Research - peer-review › Poster – Annual report year: 2017

Uncertainty and Sensitivity Analysis for an Ibuprofen Synthesis Model Based on Hoechst Path

The pharmaceutical industry faces several challenges and barriers when implementing new or improving current pharmaceutical processes, such as competition from generic drug manufacturers and stricter regulations from the U.S. Food and Drug Administration and the European Medicine agency. The demand for efficient and reliable models to simulate and design/improve pharmaceutical processes is therefore increasing. For the case of ibuprofen, a well-known anti-inflammatory drug, the existing models do not include its complete synthesis path, usually referring only to one out of a set of different reactions. To this end, we integrated different models in this work to obtain a comprehensive synthesis model for ibuprofen, in a MATLAB/Simulink model interface. The process flowsheet is based on the Hoechst path, starting from the Friedel-Crafts acetylation of isobutylbenzene to 4-isobutylphenylacetophenone, its further hydrogenation to IBPE (1,4-isobutylphenylethanol) and the carbonylation to both ibuprofen and by-products. The integration of the referred models takes into account the different solvents used in reactions, as well as the presence of by-products and the irritants. In addition, the process path takes into consideration the effects of temperature, acidity, and the choice of the catalyst. Parameter estimation and uncertainty analysis were conducted on the kinetic model parameters using experimental data available in the literature. Finally, one factor at a time sensitivity analysis in the form of deviations in the main process inputs was made, allowing the study of the system behavior and time-response. This time-response is especially characteristic of the integrated model, as it consist of a combination of continuous and batch processes. The sensitivity analysis performed gives a good indication of the model behavior for further work, such as control implementation, plant-wide optimization, or upstream and downstream process integration.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: da Conceicao Do Carmo Montes, F. (Intern), Gernaey, K. V. (Intern), Sin, G. (Intern)
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Uncertainty assessment of equations of state with application to an organic Rankine cycle

Evaluations of equations of state (EoS) should include uncertainty. This study presents a generic method to analyse EoS from a detailed uncertainty analysis of the mathematical form and the data used to obtain EoS parameter values. The method is illustrated by comparison of Soave–Redlich–Kwong (SRK) cubic EoS with perturbed-chain statistical associating fluid theory (PC-SAFT) EoS for an organic Rankine cycle (ORC) for heat recovery to power from the exhaust gas of a marine diesel engine using cyclopentane as working fluid. Uncertainties of the EoS input parameters including their corresponding correlation structure, are quantified from experimental measurements using a bootstrap method. Variance-based sensitivity analysis is used to compare the uncertainties from the departure function and the ideal-gas contribution. A Monte Carlo procedure propagates fluid parameter input uncertainty onto the model outputs. Uncertainties in the departure function (SRK or PC-SAFT EoS) dominate the total uncertainties of the ORC model output. For this application and working fluid, SRK EoS has less predictive uncertainty in the process model output than does PC-SAFT EoS, thought cannot be determined if this is due to differences in the data for parameter estimation or in the mathematical form of the EoS or both.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, National Institute of Standards and Technology, University of Virginia
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Uncertainty Analysis of Equations of State with Application to an Organic Rankine Cycle

Evaluations of equations of state (EoS) with application to process systems should include uncertainty analysis. A generic method is presented for determining such uncertainties from both the mathematical form and the data for obtaining EoS parameter values. The method is implemented for the Soave–Redlich–Kwong (SRK), the Peng–Robinson (PR) cubic EoS, and the perturbed-chain statistical associating fluid theory (PC-SAFT) EoS, as applied to an organic Rankine cycle (ORC) power system to recover heat from the exhaust gas of a marine diesel engine with cyclopentane as the working fluid. Uncertainties of the EoS input parameters, including their corresponding correlation structure, are quantified from the data using a bootstrap method. A Monte Carlo procedure propagates parameter input uncertainties onto the process output. Regressions have been made of the three cubic EoS parameters from both critical point matching and vapor pressure and density data, as used for the three PC-SAFT parameters. ORC power uncertainties of 2-5% are found for all models from the larger data sets. Mean power values for the cubic EoS are similar for both parameter regressions. The mean power from the PC-SAFT EoS is less than for the cubic EoS, with no overlap of the uncertainty distributions.
Understanding Biomass Ignition in Power Plant Mills

Converting existing coal fired power plants to biomass is a readily implemented strategy to increase the share of renewable energy. However, changing from one fuel to another is not straightforward: Experience shows that wood pellets ignite more readily than coal in power plant mills or storages. This is not very well explained by applying conventional thermal ignition theory. An experimental study at lab scale, using pinewood as an example fuel, was conducted to examine self-heating and self-ignition. Supplemental experiments were performed with bituminous coal. Instead of characterizing ignition temperature in terms of sample volume, mass-scaling seems more physically correct for the self-ignition of solids. Findings also suggest that the transition between self-heating and self-ignition is controlled both by the availability of reactive material and temperature. Comparison of experiments at 20% oxygen with those under inert atmosphere revealed two distinct pathways, pyrolysis and exothermic heterogeneous oxidation. At low temperatures and sufficient oxygen availability, heterogeneous oxidation of the solid seems to be favored over pyrolysis for wood, but not for coal. Current ignition models do not reflect the existence of these different pathways, which may be the reason behind the discrepancy between theory and observations.

Understanding N₂O formation mechanisms through sensitivity analyses using a plant-wide benchmark simulation model

In the present work, sensitivity analyses are performed on a plant-wide model incorporating the typical treatment unit of a full-scale wastewater treatment plant and N₂O production and emission dynamics. The influence of operating temperature is investigated. The results are exploited to identify the biological mechanisms responsible for N₂O emissions, TN removal efficiency, competition for oxygen among the different microbial groups and the trade-off between oxygen consumption and effluent nitrogen loading. It was found that N₂O emissions are triggered by poor oxygenation levels which cause an imbalance in the activity of NOB over the activity of AOB. As a matter of fact this imbalance leads to nitrite accumulation which in turn triggers AOB denitrification. This is particularly true at high temperatures, due to higher difference between AOB and NOB specific growth rates. At the same time, too high oxygen availability is found to inhibit heterotrophic denitrification, leading to incomplete reduction of nitrogen oxides and thereby to an accumulation of nitrous oxide. High oxygen supply is also found to worsen effluent quality via inhibition of heterotrophic denitrification. Low temperatures have shown to drastically limit aerobic AOB activity, thus compromising effluent quality. Finally, the organic biodegradable carbon surplus leaving the anoxic zone is identified to slow down NOB activity via oxygen competition with heterotrophs in the aerobic zone. With regard to the control strategy for the minimization of N₂O emissions, the ratio between nitrate produced and ammonium consumed in an aerobic zone should be considered as candidate controlled variable to check whether nitrification is complete or nitrates are building up. Oxygen availability should be regulated according to the measured controlled variable.
Univolatility curves in ternary mixtures: geometry and numerical computation

We propose a new non-iterative numerical algorithm allowing computation of all univolatility curves in homogeneous ternary mixtures independently of the presence of the azeotropes. The key point is the concept of generalized univolatility curves in the 3D state space, which allows the main computational part to be reduced to a simple integration of a system of ordinary differential equations.
Untargeted GC-MS Metabolomics Reveals Changes in the Metabolite Dynamics of Industrial Scale Batch Fermentations of Streptococcus thermophilus Broth

An industrial scale biomass production using batch or fed-batch fermentations usually optimized by selection of bacterial strains, tuning fermentation media, feeding strategy, and temperature. However, in-depth investigation of the biomass metabolome during the production may reveal new knowledge for better optimization. In this study, for the first time, the authors investigated seven fermentation batches performed on five Streptococcus thermophilus strains during the biomass production at Chr. Hansen (Denmark) in a real life large scale fermentation process. The study is designed to investigate effects of batch fermentation, fermentation time, production line, and yeast extract brands on the biomass metabolome using untargeted GC-MS metabolomics. Processing of the raw GC-MS data using PARAFAC2 revealed a total of 90 metabolites out of which 64 are identified. Partitioning of the data variance according to the experimental design was performed using ASCA and revealed that batch and fermentation time effects and their interaction term were the most significant effects. The yeast extract brand had a smaller impact on the biomass metabolome, while the production line showed no effect. This study shows that in-depth metabolic analysis of fermentation broth provides a new tool for advanced optimization of high-volume-low-cost biomass production by lowering the cost, increase the yield, and augment the product quality.
Upscaling of enzyme enhanced CO2 capture

Fossil fuels are the backbone of the energy generation in the coming decades for USA, China, India and Europe, hence high greenhouse gas emissions are expected in future. Carbon capture and storage technology (CCS) is the only technology that can mitigate greenhouse gas emissions from fossil fuel fired power by selectively capturing CO2 from flue gases. High capital and high operational costs of this process are the major obstacles of industrial implementation. In the field of CCS the chemical absorption process is the most mature technology. The use of kinetic rate promoters that enhance the mass transfer of CO2 with slow-capturing but energetically favorable solvents can open up a variety of new process options for this technology.

The ubiquitous enzyme carbonic anhydrase (CA), which enhances the mass transfer of CO2 in the lungs by catalyzing the reversible hydration of CO2, is one very promising mass transfer rate promoter for CCS. This process has been previously been tested successfully in lab scale and in some rare cases in pilot scale, but no validated process model for this technology has been published yet.

This PhD thesis presents an investigation of the feasibility of enzyme enhanced CO2 capture technology by identifying the potentials and limitations in lab and in pilot scale and benchmarking the process against proven technologies. The main goal was to derive a realistic process model for technical size absorbers with a wide range of validity incorporating a mechanistic enzyme kinetic model and validating it against in-house pilot plant experiments.

The work consisted of identifying a suitable enzyme-solvent system and the ideal process conditions by comparing mass transfer rates of different solvents and enzyme enhanced solvents in a lab scale wetted wall column. A kinetic model for the mechanistic enzyme reactions was developed for MDEA (N-methyl-diethanolamine) solutions capable of describing the mass transfer of CO2 for absorption and desorption. It incorporates the influence of all relevant process conditions for technical absorbers, such as: temperature, solvent concentration, enzyme concentration, CO2 concentration in the gas and liquid phase, as well as bicarbonate concentration in the liquid phase.

The process with enzyme enhanced MDEA was scaled up, and absorption experiments were carried out on a 10 m high pilot absorber column. The influence of enzyme concentration, column height, as well as solvent flow rates were determined for 30 wt% MDEA in over 50 runs and compared to over 30 pilot plant runs with the industrial standard solvent 30 wt% MEA (monoethanolamine) under the same process conditions. The mass transfer performance of enzyme enhanced solutions was found to be close to the industrial standard.
The pilot plant experiments could be accurately predicted with the in-house absorber column model CAPCO2 after the kinetic enzyme model from the lab experiments was implemented. The model can very accurately simulate the influence of each process parameter tested.

For targeting the thermal stability of the enzyme in desorption, an alternative low temperature process without reboiler was presented. A stripping gas carrier is utilized in this process to avoid thermal deactivation of the enzymes in the solvent regeneration; its technical feasibility was successfully tested in pilot scale desorption experiments.

The experiments at lab and pilot scale have clearly proven CA’s potential in CCS. The presented validated absorber column model together with the low temperature regeneration process can be used to simulate and optimize the enzyme enhanced CO₂ capture process and benchmark this novel technology against conventional processes.
The present study aims to apply and validate a simple model describing the forces that are built up along the dies of a pellet press matrix to the pelleting behavior of torrefied biomass. The model combines a theoretical background with the use of a single pellet press to describe the pelleting behavior of torrefied material in an industrial scale pellet mill. Wet torrefaction and dry torrefaction pretreatments are considered in the study. Both torrefaction concepts produce a fuel with enhanced properties including a lower moisture content, higher calorific value, and better friability. The fuel shows closer properties to coal and it is more economical to transport and better to store due to its hydrophobic characteristics. The goal of the present study is to allow for a fast estimation of important pelleting process parameters, to get a better understanding of the pelleting process and to avoid time consuming as well as expensive trial and error experiments.
Voltage-stabilised elastomers with increased relative permittivity and high electrical breakdown strength by means of phase separating binary copolymer blends of silicone elastomers

Increased electrical breakdown strength and increased dielectric permittivity of silicone-based dielectric elastomers are achieved by means of the addition of so-called voltage-stabilisers prepared from PDMS–PPMS copolymers as well as PDMS–PEG copolymers in order to compensate for the negative effect of softness on electrical stability of silicone elastomers. The voltage-stabilised elastomer, incorporating a high-permittivity PDMS–PEG copolymer, possesses increased relative permittivity, high electrical breakdown strength, excellent network integrity and low dielectric loss and paves the way towards specialised silicone elastomers for dielectric elastomer transducer products with inherent softness and electrical stability, and thus increased actuation at a given voltage.
Wastewater-based epidemiology to assess pan-European pesticide exposure

Human biomonitoring, i.e. the determination of chemicals and/or their metabolites in human specimens, is the most common and potent tool for assessing human exposure to pesticides, but it suffers from limitations such as high costs and biases in sampling. Wastewater-based epidemiology (WBE) is an innovative approach based on the chemical analysis of specific human metabolic excretion products (biomarkers) in wastewater, and provides objective and real-time information on xenobiotics directly or indirectly ingested by a population. This study applied the WBE approach for the first time to evaluate human exposure to pesticides in eight cities across Europe. 24 h-composite wastewater samples were collected from the main wastewater treatment plants and analyzed for urinary metabolites of three classes of pesticides, namely triazines, organophosphates and pyrethroids, by liquid chromatography-tandem mass spectrometry. The mass loads (mg/day/1000 inhabitants) were highest for organophosphates and lowest for triazines. Different patterns were observed among the cities and for the various classes of pesticides. Population weighted loads of specific biomarkers indicated higher exposure in Castellon, Milan, Copenhagen and Bristol for pyrethroids, and in Castellon, Bristol and Zurich for organophosphates. The lowest mass loads (mg/day/1000 inhabitants) were found in Utrecht and Oslo. These results were in agreement with several national statistics related to pesticides exposure such as pesticides sales. The daily intake of pyrethroids was estimated in each city and it was found to exceed the acceptable daily intake (ADI) only in one city (Castellon, Spain). This was the first large-scale application of WBE to monitor population exposure to pesticides. The results indicated that WBE can give new information about the "average exposure" of the population to pesticides, and is a useful complementary biomonitoring tool to study population-wide exposure to pesticides.

General information

State: Published
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Whole grain-rich diet reduces body weight and systemic low-grade inflammation without inducing major changes of the gut microbiome: a randomised cross-over trial

Objective To investigate whether a whole grain diet alters the gut microbiome and insulin sensitivity, as well as biomarkers of metabolic health and gut functionality. Design 60 Danish adults at risk of developing metabolic syndrome were included in a randomised cross-over trial with two 8-week dietary intervention periods comprising whole grain diet and refined grain diet, separated by a washout period of ≥6 weeks. The response to the interventions on the gut microbiome composition and insulin sensitivity as well on measures of glucose and lipid metabolism, gut functionality, inflammatory markers, anthropometry and urine metabolomics were assessed. Results 50 participants completed both periods with a whole grain intake of 179±50 g/day and 13±10 g/day in the whole grain and refined grain period, respectively. Compliance was confirmed by a difference in plasma alkylresorcinols (p<0.0001). Compared with refined grain, whole grain did not significantly alter glucose homeostasis and did not induce major changes in the faecal microbiome. Also, breath hydrogen levels, plasma short-chain fatty acids, intestinal integrity and intestinal transit time were not affected. The whole grain diet did, however, compared with the refined grain diet, decrease body weight (p<0.0001), serum inflammatory markers, interleukin (IL)-6 (p=0.009) and C-reactive protein (p=0.003). The reduction in body weight was consistent with a reduction in energy intake, and IL-6 reduction was associated with the amount of whole grain consumed, in particular with intake of rye. Conclusion Compared with refined grain diet, whole grain diet did not alter insulin sensitivity and gut microbiome but reduced body weight and systemic low-grade inflammation.

General information
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Organisations: National Food Institute, Research Group for Gut Microbiology and Immunology, Department of Bio and Health Informatics, Metagenomics, Disease Intelligence and Molecular Evolution, Department of Biotechnology and Biomedicine, Disease Systems Immunology, Department of Chemical and Biochemical Engineering, Organic Chemistry, Center for BioProcess Engineering, DTU Multi Assay Core, Research Group for Analytical Food Chemistry, Copenhagen Center for Health Technology, University of Copenhagen, Chalmers University of Technology, Chalmers University of Technology, Bispebjerg University Hospital, Herlev and Gentofte Hospital, University of Auckland
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Main Research Area: Technical/natural sciences

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ZnO as a cheap and effective filler for high breakdown strength elastomers

Cheap, high-performance dielectric elastomers are in high demand from industry concerning new products based on dielectric elastomer transducers. However, formulating an elastomer that fulfils all the requirements for dielectric elastomers is difficult and, first and foremost, not cheap. In this article, we explore the use of a cheap and abundant metal oxide filler, namely ZnO, as a filler in silicone-based dielectric elastomers. The electro-mechanical properties of the elastomer composites are investigated, and their performance is evaluated by means of figures of merit. Various commercial silicone elastomers and a self-formulated silicone elastomer are utilised as elastomer matrices, the effects of which on the final properties of the elastomer composite are investigated.
Partially fluorinated electrospun proton exchange membranes

The present invention relates to a novel porous membrane layer, to a novel method for producing a membrane, and the membranes produced by the novel method. The present invention further relates to a fuel cell comprising the porous layer, as well as any use of the porous layer in a fuel cell or in a filter. The porous membrane layer comprises a plurality of randomly oriented fibers manufactured by electrospinning, wherein the fibers comprise a graft copolymer, wherein the graft copolymer comprises a backbone and at least one side chain, wherein the backbone comprises a partially fluorinated polymer, and wherein at least one side chain of the graft copolymer comprises a polymerization product of a polymerizable proton donor group or a precursor thereof.
Diesel-soluble lignin oils and methods of their production

Solvent consumption in supercritical ethanol, propanol or butanol treatment of either refined pre-extracted lignin or comparatively impure lignin-rich solid residual from hydrothermally pretreated lignocellulosic biomass can be minimized by conducting the reaction at very high loading of lignin to solvent. Comparatively impure, crude lignin-rich solid residual can be directly converted by supercritical alcohol treatment to significantly diesel-soluble lignin oil without requirement for pre-extraction or pre-solubilisation of lignin or for added reaction promoters such as catalysts, hydrogen donor co-solvents, acids, based or H2 gas. O:C ratio of product oil can readily be obtained using crude lignin residual in such a process at levels 0.20 or lower.

General information

State: Published
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Dielectric electroactive polymer comprising an elastomeric film in the form of a gel

Use of an elastomeric film in the form of a gel, wherein said gel is a non-conductive hydrogel or organogel, as a dielectric electroactive polymer.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
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3D Printed Silicone–Hydrogel Scaffold with Enhanced Physicochemical Properties

Scaffolds with multiple functionalities have attracted widespread attention in the field of tissue engineering due to their ability to control cell behavior through various cues, including mechanical, chemical, and electrical. Fabrication of such scaffolds from clinically approved materials is currently a huge challenge. The goal of this work was to fabricate a tissue engineering scaffold from clinically approved materials with the capability of delivering biomolecules and direct cell fate. We have used a simple 3D printing approach, that combines polymer casting with supercritical fluid technology to produce 3D interpenetrating polymer network (IPN) scaffold of silicone-poly(2-hydroxyethyl methacrylate)-co-poly(ethylene glycol) methyl ether acrylate (pHEMA-co-PEGMEA). The pHEMA-co-PEGMEA IPN materials were employed to support growth of human mesenchymal stem cells (hMSC), resulting in high cell viability and metabolic activity over a 3 weeks period. In addition, the IPN scaffolds support 3D tissue formation inside the porous scaffold with well spread cell morphology on the surface of the scaffold. As a proof of concept, sustained doxycycline (DOX) release from pHEMA-co-PEGMEA IPN was demonstrated and the biological activity of released drug from IPN was confirmed using a DOX regulated green fluorescent reporter (GFP) gene expression assay with HeLa cells. Given its unique mechanical and drug releasing characteristics, IPN scaffolds may be used for directing stem cell differentiation by releasing various chemicals from its hydrogel network.

General information
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4-Hydroxybenzoic acid from hydrothermal pretreatment of oil palm empty fruit bunches - Its origin and influence on biomass conversion

An unknown major compound, characteristically occurring during processing of oil palm empty fruit bunches was identified with LC-DAD-ESI-MS/MS to be 4-hydroxybenzoic acid. Lignin from oil palm empty fruit bunches contains 4-hydroxybenzoic acid so a tempting conclusion was that the 4-hydroxybenzoic acid originated from lignin. However, another hypothesis to its origin was also tested. The route considered involves degradation of rhamnose to 5-methylfuran-2-carbaldehyde followed by reaction with formic acid. Experimental hydrothermal pretreatment of pure rhamnose in the presence of formic acid revealed that 5-methylfuran-2-carbaldehyde is in fact a degradation product from rhamnose, analogous to glucose degradation to 5-(hydroxymethyl)-2-furaldehyde. However, the subsequent step of carboxylation with formic acid to form 4-hydroxybenzoic acid was found not to take place in practice at realistic biomass hydrothermal pretreatment conditions. 5-methylfuran-2-carbaldehyde only differs from furfural by having an extra methyl group and the degradation route indicates that it may be a new important degradation compound to consider in other biomass feedstocks rich in deoxysugars such as rhamnose or fucose, e.g. pectin rich biomasses. Assessment of the influence of 4-hydroxybenzoic acid in the enzymatic hydrolysis of pretreated oil palm empty fruit bunches as well as its presence during fermentation showed that 4-hydroxybenzoic acid is not inhibiting or mediating neither on the enzymatic hydrolysis or fermentation in the quantified range from 0.1 g/L to 1 g/L, indicating an option for reaping the 4-hydroxybenzoic acid from the biomass liquor directly after hydrothermal pretreatment for biorefinery value-addition. (C) 2016 Elsevier Ltd. All rights reserved.

General information
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Lignin, 5-Methylfuran-2-carbaldehyde, Reaction mechanism, Degradation compound, Pectin
A case study on robust optimal experimental design for model calibration of ω-Transaminase

Proper calibration of models describing enzyme kinetics can be quite challenging. This is especially the case for more complex models like transaminase models (Shin and Kim, 1998). The latter fitted model parameters, but the confidence on the parameter estimation was not derived. Hence, the usability of the parameter estimates is difficult to assess. In this paper, the confidence is derived, using the Fisher Information Matrix (FIM) for the backward reaction (conversion of acetophenone and alanine to o-methylbenzylamine and pyruvate). FIM computation requires local parameter sensitivities and measurement errors. Since the latter was not provided, a conservative standard deviation of 5% was assumed. The confidence analysis yielded that only two (Vr and Kac) out of five parameters were reliable estimates, which means that model predictions and decisions based on them are highly uncertain. The reason behind this problem is practical identifiability, which can be related to both the model structure and/or the information content of the data. The available data are 25 experiments performed by Shin and Kim, set up in a 5x5 factorial design (2 substrates with 5 concentration levels each) across the experimental space. However, it is expected that more informative experiments can be designed to increase the confidence of the parameter estimates. Therefore, we apply Optimal Experimental Design (OED) to the calibrated model of Shin and Kim (1998). The total number of samples was retained to allow fair comparison with the original experimental design. Using OED led to unique and higher quality parameter estimates for all parameters. This illustrates that OED can increase parameter confidence without increasing the experimental effort. The main problem which arises when performing OED is that the "real" parameter values are not known before finishing the model calibration. However, it is important that the chosen parameter values are close to the real parameter values, otherwise the OED can possibly yield non-informative experiments. To counter this problem, one can use robust OED. The idea of robust OED is to make the design less dependent on one specific parameter set, but make it suitable for a subset of parameters in a local parameter space. This robust OED methodology is currently being applied to the backward part of the model of Shin and Kim (1998) to design experiments for the conversion of 1-methyl-2-phenylpropylamine and acetone to benzylacetone and isopropylamine and yield a reliable estimation for all parameters. Details of the outcome will be shown at the conference.

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Acceleration of Anti-Markovnikov Hydroamination in the Synthesis of an Active Pharmaceutical Ingredient

Slow chemical reactions are a big challenge in the modern pharmaceutical industry. Their accelerations together with the introduction of continuous manufacturing modes are major drivers for future development. One example reaction is hydroamination, a reaction between unsaturated hydrocarbons and amines. Such a reaction type is the main focus of this work. More precisely, the anti-Markovnikov hydroamination reaction between cis/trans 9H-thioxanthene-2-chloro-9-(2-propenylidene)-(9CI) and 1-(2-hydroxyethyl)piperazine (HEP) is investigated in detail. It has been traditionally performed in toluene with a huge excess of HEP and reaction times of up to 24h. Acceleration of the reaction from 24 down to 4h is achieved by switching from batch operation mode in toluene to either solvent-free batch mode or microwave-assisted hydroamination with tetrahydrofuran as a solvent.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CHEC Research Centre, H. Lundbeck A/S
Authors: Mitic, A. (Intern), Skovby, T. (Ekstern), Dam-Johansen, K. (Intern), Gernaey, K. (Intern)
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Publication date: 2016
Main Research Area: Technical/natural sciences
A CFD model for determining mixing and mass transfer in a high power agitated bioreactor
Prediction of mixing and mass transfer in agitated systems is a vital tool for process development and scale up in industrial biotechnology. In particular key process parameters such as mixing time and kLa are essential for bioprocess development [1]. In this work the mixing and mass transfer performance of a high power agitated pilot scale bioreactor has been characterized using a novel combination of computational fluid dynamics (CFD) and experimental investigations. The effect of turbulence inside the vessel was found to be most efficiently described by using the k-ε model with regards to computational effort and required accuracy for industrial application. Mixing time was determined by carrying out sodium chloride tracer experiments at various bulk viscosities and agitation speeds, while tracking the conductivity. The mixing performance was predicted with one-phase CFD simulations and showed good agreement with the experimental data. The mass transfer coefficient was determined during three fed batch Trichoderma reesei fermentations at different process conditions previously described in [2]. Similarly the mass transfer was predicted by Higbie’s penetration model [3] from two-phase CFD simulations, and the overall mass transfer coefficient was found to be in accordance with experimental data. This work illustrates the possibility of predicting the hydrodynamic performance of an agitated bioreactor using validated CFD models. These models can be applied in the testing of new bioreactor configurations, and to illustrate the effect of changing the physical process conditions. This is a showcase of how we have expanded our work in the area of mixing from microscale reactors to pilot scale industrial systems and we would like to present this work in order to receive feedback.

Acidic-alkaline ferulic acid esterase from Chaetomium thermophilum var. dissitum: Molecular cloning and characterization of recombinant enzyme expressed in Pichia pastoris
A novel ferulic acid esterase encoding gene CtFae, was successfully cloned from a highly esterase active strain of the thermophile ascomycetous fungus Chaetomium thermophilum var. dissitum; the gene was heterologously expressed in Pichia pastoris KM71H. The recombinant enzyme (CtFae) was purified to homogeneity and subsequently characterized. CtFae was active towards synthetic esters of ferulic, p-coumaric, andcaffeic acids, as well as towards wide range of p-nitrophenyl substrates. Its temperature and pH optima were 55 °C and pH 6.0, respectively. Enzyme rare features were broad pH optimum, high stability at extended acidic-alkaline pH region, and noticeable thermostability. CtFae released ferulic acid from wheat insoluble arabinoxylan, as well as ferulic and p-coumaric acids from wheat straw and ryegrass, indicating potentials for industrial applications like biomass conversion in biorefineries.
A collocation method for surface tension calculations with the density gradient theory

Surface tension calculations are important in many industrial applications and over a wide range of temperatures, pressures and compositions. Empirical parachor methods are not suitable over a wide condition range and the combined use of density gradient theory with equations of state has been proposed in literature. Often, many millions of calculations are required in the gradient theory methods, which is computationally very intensive. In this work, we have developed an algorithm to calculate surface tensions an order of magnitude faster than the existing methods, with no loss of accuracy. The new method can be used with any equation of state, and gives much improved performance. In this work, the new method for solving the gradient density theory equations is combined with cubic equations of state and the Cubic-Plus-Association model. Applications for both binary and multicomponent mixtures and for both hydrocarbon and associating systems are shown. For most systems, the predictions obtained are in good agreement with experimental data. However, cases have been identified where further investigation is needed.

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BFI (2012): BFI-level 2
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BFI (2011): BFI-level 2
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ISI indexed (2011): ISI indexed yes
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A comment on water’s structure using monomer fraction data and theories

Monomer fraction data for water (and other compounds) can provide useful information about their structure and can be used in “advanced” equations of state, which account explicitly for association phenomena. Recent findings about the performance of association theories in representing the monomer fraction of water are reviewed. Three such theories are considered and all of them perform qualitatively similar. They can all represent phase equilibria for water solutions qualitatively well but with parameters which are not in good agreement with Luck’s famous monomer fraction data. While this could set the theoretical basis of these theories in doubt, we also show in this work that the findings with these association models are in agreement with a recently presented theory which links monomer fraction to dielectric constants. This new theory, like the three thermodynamic models, predicts more hydrogen bonding in water than Luck’s data (Angew. Chem. Int. Ed. Engl. 1980, vol. 19, pp. 28). Moreover, it appears that both the new theory and the three models provide evidence for the four-site association scheme for water and thus support that the tetrahedral structure of the water molecule is correct or at least that the tetrahedral structure is in agreement with several pure water physical properties, monomer fraction information and phase equilibria data in mixtures with alkanes.

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Authors: Liang, X. (Intern), Maribo-Mogensen, B. (Intern), Tsivintzelis, I. (Intern), Kontogeorgis, G. M. (Intern)
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A comparison of partially acetylated nanocellulose, nanocrystalline cellulose, and nanoclay as fillers for high-performance polylactide nanocomposites

Partially acetylated cellulose nanofibers (CNF) were chemically extracted from sisal fibers and the performance of those CNF as nanofillers for polylactide (PLA) for food packaging applications was evaluated. Three PLA nanocomposites; PLA/CNF (cellulose nanofibers), PLA/CNC (nanocrystalline cellulose), and PLA/C30B (CloisiteTM 30B, an organically modified montmorillonite clay) were prepared and their properties were evaluated. It was found that CNF reinforced composites showed a larger decrease on oxygen transmission rate (OTR) than the clay-based composites; (PLA/CNF 1% nanocomposite showed a 63% of reduction at 238C and 50% RH while PLA/C30B 1% showed a 26% decrease) and similar behavior on terms of water vapor barrier properties with 46 and 43%, respectively of decrease on water vapor transmission rate at 238C and 50% RH (relative humidity). In terms of mechanical and thermomechanical properties, CNF-based nanocomposites showed better performance than clay-based composites without affecting significantly the optical transparency.
A Comprehensive Methodology for Development, Parameter Estimation, and Uncertainty Analysis of Group Contribution Based Property Models – An Application to the Heat of Combustion

A rigorous methodology is developed that addresses numerical and statistical issues when developing group contribution (GC) based property models such as regression methods, optimization algorithms, performance statistics, outlier treatment, parameter identifiability, and uncertainty of the prediction. The methodology is evaluated through development of a GC method for the prediction of the heat of combustion (ΔHco) for pure components. The results showed that robust regression lead to best performance statistics for parameter estimation. The bootstrap method is found to be a valid alternative to calculate parameter estimation errors when underlying distribution of residuals is unknown. Many parameters (first, second, third order group contributions) are found unidentifiable from the typically available data, with large estimation error bounds and significant correlation. Due to this poor parameter identifiability issues, reporting of the 95% confidence intervals of the predicted property values should be mandatory as opposed to reporting only single value prediction, currently the norm in literature. Moreover, inclusion of higher order groups (additional parameters) does not always lead to improved prediction accuracy for the GC-models; in some cases, it may even increase the prediction error (hence worse prediction accuracy). However, additional parameters do not affect calculated 95% confidence interval. Last but not least, the newly developed GC model of the heat of combustion (ΔHco) shows predictions of great accuracy and quality (the most datafalling within the 95% confidence intervals) and provides additional information on the uncertainty of each prediction compared to other ΔHco models reported in literature.

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A Correlation between the Activity of Candida antarctica Lipase B and Differences in Binding Free Energies of Organic Solvent and Substrate

The ability of enzymes to operate in organic solvent is now widely accepted and is the basis for extensive research in enzymology. The challenge is to select the solvent media that allows the modulation of enzyme activity. For a rational selection of a solvent, it is necessary to understand the effect of organic solvent molecules on enzyme structure and the enzymatic reaction on a molecular level. To gain such insight, we combined experimental kinetics studies with full atomic molecular dynamics simulations and found a correlation between the activity of Candida antarctica lipase B (CALB) [for the esterification reaction between butyric acid and ethanol at a fixed water activity] and the binding of the solvent/substrate molecules in the active site region of CALB. We have investigated the influence of four organic solvents hexane (HEX), methyl tertiary butyl ether (MTBE), acetonitrile (ACN), and tertiary butanol (TBU)-on the catalytic activity of CALB for the esterification reaction. The solvents have been chosen on the basis of different polarity-functional groups. Our study shows that these organic solvents do not alter the overall conformation of CALB; rather, the solvent effects on the performance of the enzyme may be ascribed to binding of solvent molecules to the enzyme active site region and the solvation energy of substrate molecules in the different solvents. Polar solvent molecules interact strongly with CALB and compete with the substrate to bind to the active site region, resulting in an inhibitory effect which is also confirmed by the binding free energies for the solvent and substrate molecules estimated from the simulations. Consequently, the catalytic activity of CALB decreases in polar solvents. This effect is significant, and CALB is over 10 orders of magnitude more active in nonpolar solvents (HEX and MTBE) than in the polar solvents (ACN and TBU). TBU molecules show an exceptional behavior because the solvent molecule forms an extensive hydrogen bond network within the CALB active site region suggesting that solvent molecules rich on hydrogen bond acceptors and donors are poor solvents when used for lipase-catalyzed esterification reactions.
Active Disturbance Rejection Control of a Heat Integrated Distillation Column

Heat integrated distillation column (HiDC) is the most energy efficient distillation approach making efficient utilization of internal heat integration through heat pump. The rectifying section acts as a heat source with high pressure, while the stripping section operates as a heat sink with low pressure. However, the control of some HiDC processes is generally difficult due to the strong control loop interaction, high purity of the components and undesired disturbances. Active disturbance rejection control (ADRC) is used in this paper to control a simulated HiDC for separating benzene-toluene mixture. The efficiency of the ADRC technique is demonstrated by comparing with the conventional PI controller in terms of set-point tracking and external disturbance rejection capability. The results show that the ADRC gives much improved control performance than the PID control.

A density gradient theory based method for surface tension calculations

The density gradient theory has been becoming a widely used framework for calculating surface tension, within which the same equation of state is used for the interface and bulk phases, because it is a theoretically sound, consistent and computationally affordable approach. Based on the observation that the optimal density path from the geometric mean density gradient theory passes the saddle point of the tangent plane distance to the bulk phases, we propose to estimate surface tension with an approximate density path profile that goes through this saddle point. The linear density gradient theory, which assumes linearly distributed densities between the two bulk phases, has also been investigated. Numerical problems do not occur with these density path profiles. These two approximation methods together with the full density gradient theory have been used to calculate the surface tension of various systems, from non-polar binary mixtures to complex multicomponent associating fluids, combined with the Peng-Robinson and the Cubic Plus Association equations of state. From an overall point of view, the approximation method with the density path profile passing the saddle point and the full density gradient theory offer comparable performance in predicting surface tension, while the linear density
gradient theory frequently overpredicts. Limitations have been seen for all the three methods in correlating the surface
tension of particular systems, with a single adjustable parameter for the cross influence parameter.
Adhesion Strength of Biomass Ash Deposits

Ash deposition on boiler surfaces is a major problem encountered during biomass combustion. Ash deposition adversely influences the boiler efficiency, may corrode heat transfer surfaces, and may even completely block flue gas channels in severe cases, causing expensive unscheduled boiler shutdowns. Therefore, timely removal of ash deposits is essential for optimal boiler operation. In order to improve the qualitative and quantitative understanding of deposit shedding in boilers, this study investigates the shear adhesion strength of biomass ash deposits on superheater tubes. Artificial biomass ash deposits were prepared on superheater tubes and sintered in an oven at temperatures up to 1000 °C. Subsequently, the deposits were sheared off by an electrically controlled arm, and the corresponding adhesion strength was measured. The results reveal the effect of temperature, ash/deposit composition, sintering duration, and steel type on the adhesion strength.

General information

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Advances in European cord wood testing and policy

Wood stoves have the potential of providing CO₂ neutral energy without transmission loss—but with the significant drawbacks of high emissions of pollutants and particulate matter at low altitude close to private homes, and with an uneven heat release profile, which produces non-optimal heating comfort.A collaboration project between the CHEC research centre at DTU Chemical Engineering and the stove manufacturing company HWAM A/S has led to development of an automatic control system forwood stoves, and the first version of an automatically controlled wood stove was launched on the market in 2012. The automatic control system developed for wood stoves in this project ensures optimal combustion conditions, thereby minimizing the emissions throughout a complete wood log combustion cycle. This improved performance has been verified by field tests in private homes.
A Dynamic Design Space for Primary Drying During Batch Freeze-Drying

Biopharmaceutical products are emerging within the pharmaceutical industry. However, biopharmaceuticals are often unstable in aqueous solution. Freeze-drying (lyophilisation) is the preferred method to achieve a stable product with an increased shelf-life. During batch freeze-drying, there are only two adaptable process variables, i.e. the shelf temperature and the pressure in the drying chamber. The value of both should be optimized, preferably in a dynamic way, to minimise the primary drying time while respecting process and equipment constraints and ensuring end product quality. A mechanistic model is used to determine the optimal values for the adaptable variables, hereby accounting for the uncertainty in all involved model parameters. A dynamic Design Space was constructed with a risk of failure acceptance level of 0.01%, i.e. a ‘zero-failure’ situation. Even for a risk of failure of 0.01%, the computed settings resulted in a reduction of the drying time by over 50% compared to current practice.
A flexible well-mixed milliliter-scale reactor with high oxygen transfer rate for microbial cultivations

In order to choose the best strain and subsequently develop an optimal bioprocess many experiments need to be performed. Usually this process is expensive and labor intensive with a limited amount of data available. Small-scale bioreactors and high-throughput platforms are becoming an attractive solution and replacement for existing microtiter plates, shaken flasks and bench scale bioreactors. In this work, a new design of a milliliter-scale bioreactor system is presented and characterized. The entire system consists of a platform with gas connections, heater, temperature sensor and optical fibers on the one side and a bioreactor with special designed magnetic stirrer and non-invasive optical sensors for measurement of pH, dissolved oxygen and optical density on the other side. The system has a high level of flexibility in terms of volume (0.5–2 mL), aeration (sparging and surface aeration) and mixing (one- and bi-directional). Computational fluid dynamics (CFD) was employed in order to simulate the mixing times, the oxygen transfer rates and the appearance and size of the gas-liquid interfaces in the 1 mL-scale bioreactor with unidirectional mixing and surface aeration. Mixing performance was tested and the oxygen transfer rate was determined experimentally as well. The obtained results show a good mixing time (between 0.4 s and 2 s) and a high oxygen transfer rate ($k_{L}a > 1000 \text{ h}^{-1}$). The milliliter-scale bioreactor platform was used to cultivate Saccharomyces cerevisiae and Lactobacillus paracasei.
A framework for techno-economic & environmental sustainability analysis by risk assessment for conceptual process evaluation

The need to achieve a sustainable process performance has become increasingly important in order to keep a competitive advantage in the global markets. Development of comprehensive and systematic methods to accomplish this goal is the subject of this work. To this end, a multi-level framework for techno-economic and environmental sustainability analysis through risk assessment is proposed for the early-stage design and screening of conceptual process alternatives. The alternatives within the design space are analyzed following the framework’s work-flow, which targets the following: (i) quantify the economic risk; (ii) perform the monetary valuation of environmental impact categories under uncertainty; (iii) quantify the potential environmental risk; (iv) measure the alternatives’ eco-efficiency identifying possible trade-offs; and, lastly (v) propose a joint risk assessment matrix for the quantitative and qualitative assessment of sustainability at the decision-support level. Through the application of appropriate methods in a hierarchical manner, this tool leads to the identification of the potentially best and more sustainable solutions. Furthermore, the application of the framework is highlighted by screening two conceptual glycerol bioconversion routes to value-added chemicals namely 1,3-propanediol.
(1,3-PDO) and succinic acid.

**General information**

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A Generic Methodology for Superstructure Optimization of Different Processing Networks

A large focus is placed on sustainability and sustainable practices as a result of the arising environmental issues. As an element of this, sustainable process synthesis and design becomes important. A generic, systematic methodology is proposed for solving the problem of optimal design of sustainable processing networks containing three stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. In this work, a focus is placed on the first stage, the synthesis stage. Process synthesis becomes necessary in determining the appropriate processing routes to produce a selection of products from a set or feedstock. The problem to be solved here is the following: for a given set of raw materials, products and a network of processing routes, determine the optimal processing route from a sustainability point of view. Three different processing networks arising from chemical processes, biorefineries, and carbon dioxide utilization are considered. In the synthesis stage, the processing alternatives are represented in a superstructure and the associated data is collected and stored in a database. Once a specific process synthesis problem is formulated, the existing superstructure is retrieved and reduced in order to include only the relevant alternatives. New alternatives can easily be added and stored in the database. The superstructure of alternatives in the network is then represented using a generic data-independent process model, which yields a mixed integer linear or nonlinear programming problem. The proposed methodology involves the use of additional methods and tools, such as a database and an external software for solving the network optimization problem. The database has been created using an ontology-based knowledge representation consisting in various layers of data and interconnections between them. Using a common database structure for any process synthesis problem allows for easy data collection, storage and retrieval, as well as giving the possibility of solving combined problems that have been previously solved independently. The step-by-step methodology has been implemented in a software interface that guides the user through the problem formulation and solution steps and integrates the various methods and tools for efficient flow of information between them. By using this interface, the user can retrieve and/or modify existing networks and alternatives from the database, as well as add new alternatives and connections between them. With the generated superstructure of alternatives and the corresponding data, an input file for GAMS is
A generic methodology for the design of sustainable carbon dioxide utilization processes using superstructure optimization

Global warming and other environmental concerns are fueling increased focus on sustainability resulting in new and stringent guidelines, especially with regard to emissions [1]. Greenhouse gases are prevalent and among harmful emissions that are targeted to be reduced; carbon dioxide (CO2) is the primary greenhouse gas that is targeted via carbon capture and storage (CCS) as well as carbon capture and utilization (CCU) [1]. Carbon capture and utilization is showing promise because, in contrast with carbon capture and storage, it takes the captured carbon dioxide and makes further use of it, including as an extractive agent or raw material. Chemical conversion, an important element of utilization, involves the use of carbon dioxide as a reactant in the production of chemical compounds [2]. However, for feasible implementation, a systematic methodology is needed for the design of the utilization, especially chemical conversion, processes. To achieve this, a generic methodology has been developed, which adopts a three-stage approach consisting in (i) process synthesis, (ii) process design, and (iii) innovative and sustainable design [3]. This methodology, with the individual steps and associated methods and tools, has been developed and applied to carbon dioxide utilization networks.

This work will focus on the first stage, process synthesis, of this three-stage methodology; process synthesis is important in determining the appropriate processing route to produce products from a selection of feedstock [4], in this case carbon dioxide. This stage contains three steps, each incorporating relevant methods and tools. First, with the help of user specifications, the problem is specified. Then, the processing routes linking feed and product are represented via a superstructure. This is performed with the help of a software interface, Super-O, guiding through the steps of the methodology related to superstructure development and optimization [5]. The data necessary to perform this step is extracted from an especially structured database ontologically designed for the easy extraction and addition of data. This database contains information on the raw material (including different carbon dioxide emission conditions), the products and the reactions linking these. With this help of the database it is possible to quickly compare utilization processes for a specific problem as the information is easily accessible; thereby, for the problem of certain products and given a specific feed it becomes easy to say which conversion processes are most promising to sustainably reduce emissions.

This methodology, the software interface and the database will be presented together with validation results from a conceptual example. Using the methodology a network of conversion reactions from carbon dioxide to various carbon, hydrogen and oxygen containing compounds, such as methanol, dimethyl ether and dimethyl carbonate, is developed; using ProCARP [6], a software tool for reaction path synthesis, the network is created containing the feasible reactions. Using the developed database, the data needed, including reaction conversions and separation factors, for the superstructure is extracted. The optimization gives the selection of the best processing routes. These are subsequently designed rigorously and analyzed for economic and environmental sustainability. The resulting design and analysis show the use of the methodology and the opportunity for sustainable reduction of emissions using conversion processes to produce chemical products.
A generic model-based methodology for quantification of mass transfer limitations in microreactors

Microreactors are becoming more popular in the biocatalytic field to speed up reactions and thus achieve process intensification. However, even these small-scale reactors can suffer from mass transfer limitations. Traditionally, dimensionless numbers such as the second Damköhler number are used to determine whether the reaction is either kinetically or mass transfer limited. However, these dimensionless numbers only give a qualitative measure of the extent of the mass transfer limitation, and are only applicable to simple reactor configurations. In practice, this makes it difficult to rapidly quantify the importance of such mass transfer limitations and compare different reactor configurations. This paper presents a novel generic methodology to quantify mass transfer limitations. It was applied to two microreactor configurations: a microreactor with immobilised enzyme at the wall and a Y-shaped microreactor with one inlet stream containing enzyme and the other containing substrate. The results of the immobilised enzyme microreactor correspond very well with the traditional approach of using the second Damköhler number (DaII). However, the results of the Y-shaped microreactor showed that the second Damköhler number is not applicable in this case, indicating that dimensionless numbers should be applied with care. For both configurations, the mass transfer limitations could be quantified and linked with appropriate dimensionless numbers, illustrating the power of the proposed methodology.

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Waste-derived fuels, such as solid recovered fuel (SRF), are increasingly being used in, e.g., the cement industry as a means to reduce cost. The inhomogeneous nature of SRF makes it difficult to combust, and many problems may arise within, e.g., combustion control, feeding of fuel, deposit formation, or accumulation of impurities. The combustion of polyethylene (PE), polypropylene (PP), polyethylene terephthalate (PET), wood, and SRF were studied in a rotary drum furnace. The combustion was recorded on a camera (60 frames per second), so that any agglomeration or deposition of fuel or ash could be monitored. PE and PP pose no significant risk of forming deposits in a combustion environment (T > 800 °C) as a result of a rapid devolatilization, while PET may cause deposits as a result of a sticky char residue. The deposition tendency of the investigated SRF is low, and it may be managed by a careful combustion control. The ash from SRF or wood does not pose a significant risk of melting and deposits at temperatures up to 1000 °C, but the presence of glass impurities in some SRF may limit operation temperatures to 900 °C as a result of ash melting.

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Web of Science (2015): Indexed yes  
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A grand model for chemical product design

Chemical engineering has been expanding its focus from primarily business-to-business products (B2B) to business-to-consumer (B2C) products. The production of B2B products generally emphasizes on process design and optimization, whereas the production of B2C products focuses on product quality, ingredients and structure. Market and competitive analysis, government policies and regulations have to be explicitly considered in product design. All these considerations are accounted for in the Grand Product Design Model, which consists of a process model, a property model, a quality model, a cost model, a pricing model, an economic model as well as factors such as company strategy, government policies and regulations. This article introduces the model and highlights selected aspects of the model with two case studies. One is a die attach adhesive that illustrates how pricing affects profitability, and how product composition changes with market conditions. Another is a hand lotion that illustrates how product quality affects the profit. (C) 2016 Elsevier Ltd. All rights reserved.
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<td>1999</td>
<td>BFI-level 2</td>
<td>Indexed yes</td>
<td>SJR 1.073 SNIP 1.113</td>
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Product design, Product ingredients, Product structure, Product price, Government policies

DOIs:
A Layout for the Carbon Capture with Aqueous Ammonia without Salt Precipitation

Post-combustion carbon capture technologies seem to be necessary to realize the CO2 mitigation policies internationally shared for the next future, despite none of them appears to be ready for full-scale applications. This work considers the aqueous ammonia based process for a coal-fired Ultra Super Critical power plant. Two layouts are simulated with Aspen Plus employing the recently recalibrated Extended UNIQUAC thermodynamic model. The first one operates at chilling conditions, which yield to salt precipitation, and is taken as reference because already analyzed in previous studies. The second layout operates at cooled conditions, which does not yield any salt precipitation. The Chilled layout reveals low specific heat duty and SPECCA equal to 2.2 and 2.86 MJ/kgco2, respectively. In contrast, the Cooled layout presents a higher specific heat duty of almost 3 MJ/kgco2 but, importantly, a lower SPECCA of 2.58 MJ/kgco2. The latter layout is a better choice also from the perspective of the plant operation since it does not present the salt precipitation.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Politecnico di Milano
Authors: Bonalumi, D. (Ekstern), Valenti, G. (Ekstern), Lillia, S. (Ekstern), Fosbøl, P. L. (Intern), Thomsen, K. (Intern)
Pages: 134-143
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.16 SJR 0.467 SNIP 0.586
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.365 SNIP 0.561 CiteScore 0.92
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.433 SNIP 0.81 CiteScore 1.09
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.425 SNIP 0.785 CiteScore 1.02
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.433 SNIP 0.957
Web of Science (2009): Indexed yes
Original language: English
CO2 capture, Carbon capture, Aqueous ammonia, Salt precipitation

Electronic versions:
A_Layout_for_the_Carbon_Capture_with_Aqueous_Ammonia_without_Salt_Precipitation.pdf

DOIs:
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Bibliographical note
This is an open access article
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A methodological approach to the design of optimising control strategies for sewer systems

This study focuses on designing an optimisation based control for sewer system in a methodological way and linking it to a regulatory control. Optimisation based design is found to depend on proper choice of a model, formulation of objective function and tuning of optimisation parameters. Accordingly, two novel optimisation configurations are developed, where the optimisation either acts on the actuators or acts on the regulatory control layer. These two optimisation designs are evaluated on a sub-catchment of the sewer system in Copenhagen, and found to perform better than the existing control; a rule based expert system. On the other hand, compared with a regulatory control technique designed earlier in Mollerup et al. (2015), the optimisation showed similar performance with respect to minimising overflow volume. Hence for operation of small sewer systems, regulatory control strategies can offer promising potential and should be considered along more advanced strategies when identifying novel solutions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering, Urban Water Systems
Authors: Mollerup, A. L. (Intern), Mikkelsen, P. S. (Intern), Sin, G. (Intern)
Pages: 103-115
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Environmental Modelling & Software
Volume: 83
ISSN (Print): 1364-8152
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.8 SJR 1.936 SNIP 2.112
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.119 SNIP 2.172 CiteScore 4.67
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.065 SNIP 2.483 CiteScore 5.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.082 SNIP 2.458 CiteScore 4.8
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.829 SNIP 2.012 CiteScore 3.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.68 SNIP 2.096 CiteScore 3.52
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.684 SNIP 2.221
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.965
BFI (2008): BFI-level 2
A methodological framework for the development of feasible CO₂ conversion processes
Converting captured CO₂ feedstock into valuable chemical products is viewed as one of the potential ways to reduce atmospheric CO₂ emission. To this end, a methodological framework is suggested to support the development of feasible CO₂ conversion processes that can contribute to the CO₂ reduction by replacing non-CO₂ utilizing processes or non CO₂-based products. The framework encompasses several execution and decision steps and uses three main criteria, which are the demand availability, CO₂ reduction feasibility, and economic feasibility. As an illustrative example, a methanol plant employing combined reforming (CR) of methane reaction is developed. To supply the CO₂ feedstock, the aMDEA-based CO₂ capture applied to a SMR-based H₂ plant is considered. A baseline process is developed and is compared with a non-CO₂ utilizing conventional methanol plant (process substitution) and a gasoline production process (product substitution) in terms of the established criteria. For the former, it is verified that the methanol production via combined reforming leads to cheaper unit production cost as well as lower net CO₂ emission compared to the conventional methanol plant. For the latter, it is shown that the feasibility of the CO₂-based methanol as an alternative fuel to gasoline highly depends on the type and price of the raw materials. To improve the developed baseline CO₂ conversion process further, (1) some of the combined reforming reaction related design variables are fine-tuned using a sensitivity analysis and an equilibrated syngas plot, and (2) utilization of various renewable energy resources for the internal electricity demand is examined.

General information
State: Published
Organisations: CAPEC-PROCESS, Department of Chemical and Biochemical Engineering, Korea Advanced Institute of Science & Technology
Authors: Roh, K. (Ekstern), Lee, J. H. (Ekstern), Gani, R. (Intern)
Pages: 250-265
Publication date: 2016
Main Research Area: Technical/natural sciences

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Volume: 47
ISSN (Print): 1750-5836
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.38 SJR 1.345 SNIP 1.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.515 SNIP 1.537 CiteScore 4.37
BFI (2014): BFI-level 1
This work presents a systematic methodology that has been developed for the design of sustainable CO\textsubscript{2} utilization processes that can mitigate CO\textsubscript{2} and also guarantee profitability. First, the three-stage methodology, evaluation criteria and applicable tools are described. Especially, the process design and analysis is discussed as only limited amounts of process data is available for determining the optimal processing path and in the third stage the issue of implementation strategy is considered. As examples, two CO\textsubscript{2} utilization methods for methanol production, combined reforming and direct synthesis are considered. Methanol plants employing such methods are developed using synthesis-design and simulation tools and their evaluation indicators are calculated under various implementation strategies. It is demonstrated that integrating or replacing an existing conventional methanol plant by a combined reforming method represents a sustainable solution. Additionally, producing methanol through direct hydrogenation is a promising way to convert CO\textsubscript{2} when cheap H\textsubscript{2} feeds are available.
A microfluidic toolbox for the development of in-situ product removal strategies in biocatalysis

A microfluidic toolbox for accelerated development of biocatalytic processes has great potential. This is especially the case for the development of advanced biocatalytic process concepts, where reactors and product separation methods are closely linked together to intensify the process performance, e.g., by the use of in-situ product removal (ISPR). This review provides a general overview of currently available tools in a microfluidic toolbox and how this toolbox can be applied to the development of advanced biocatalytic process concepts. Emphasis is placed on describing the possibilities and advantages of the microfluidic toolbox that are difficult to achieve with conventional batch-process-based technologies. Application of this microfluidic toolbox will potentially make it possible to intensify biocatalytic reactions and thereby facilitate the development towards novel and advanced biocatalytic processes, which in many cases have proven too difficult in conventional batch equipment.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Heintz, S. (Intern), Mitic, A. (Intern), Ringborg, R. H. (Intern), Krühne, U. (Intern), Woodley, J. (Intern), Gernaey, K. (Intern)
Pages: 18–26
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Flow Chemistry
Volume: 6
Issue number: 1
ISSN (Print): 2062-249X
Ratings:
Web of Science (2018): Indexed yes
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.54 SJR 0.596 SNIP 0.335
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.493 SNIP 0.437 CiteScore 1.62
Scopus rating (2014): SJR 0.501 SNIP 0.509 CiteScore 1.75
Scopus rating (2013): SJR 0.759 SNIP 0.379 CiteScore 1.7
Scopus rating (2012): SJR 0.688 SNIP 0.586
Original language: English
Microfluidics, In-situ product removal (ISPR), Process intensification, Biocatalysis, Process development
Electronic versions:
Heintz_2016.pdf
DOI:
10.1556/1846.2015.00040
Source: PublicationPreSubmission
Source-ID: 123936134
Publication: Research - peer-review › Review – Annual report year: 2016

Amino-Functional Polybenzimidazole Blends with Enhanced Phosphoric Acid Mediated Proton Conductivity as Fuel Cell Electrolytes

A new amino-functional polybenzimidazole copolymer is synthesized by homogeneous solution condensation polymerization from a novel monomer, N,N'-bis (2,4-diaminophenyl)-1,3-diaminopropane. The copolymer readily dissolves in organic solvents and shows good film forming characteristics. To balance the phosphoric acid uptake and to obtain mechanically robust membranes, the amino-functional polybenzimidazole derivative is blended with high molecular weight poly [2,2′-(m-phenylene)-5,5′-bisbenzimidazole] at different ratios. Due to the high acid uptake, the homogenous blend membranes show enhanced proton conductivity at temperatures well above 100 °C as also confirmed by the fuel cell polarization data.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Aili, D. (Intern), Javakhishvili, I. (Intern), Han, J. (Intern), Jankova Atanasova, K. (Intern), Pan, C. (Intern), Hvilsted, S. (Intern), Jensen, J. O. (Intern), Bjerrum, N. J. (Intern), Li, Q. (Intern)
Pages: 1161-1168
Publication date: 2016
Main Research Area: Technical/natural sciences
Publication information
Journal: Macromolecular Chemistry and Physics
Volume: 217
Issue number: 10
ISSN (Print): 1022-1352
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.58 SJR 0.949 SNIP 0.728
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.942 SNIP 0.79 CiteScore 2.56
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.956 SNIP 0.774 CiteScore 2.48
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.911 SNIP 0.813 CiteScore 2.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.008 SNIP 0.794 CiteScore 2.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.019 SNIP 0.793 CiteScore 2.33
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.208 SNIP 0.874
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Scopus rating (2009): SJR 1.429 SNIP 0.845
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.216 SNIP 0.823
Web of Science (2008): Indexed yes
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Scopus rating (2006): SJR 1.359 SNIP 0.978
Scopus rating (2005): SJR 1.133 SNIP 0.946
Scopus rating (2004): SJR 0.992 SNIP 0.902
Scopus rating (2003): SJR 0.932 SNIP 0.825
Scopus rating (2002): SJR 1.137 SNIP 0.837
Scopus rating (2001): SJR 1.427 SNIP 1.161
Scopus rating (2000): SJR 1.29 SNIP 1.151
Scopus rating (1999): SJR 1.524 SNIP 1.24
Original language: English
Electronic versions:
Post_print_Amino_Functional_Polybenzimidazole_Blends_with_Enhanced_Phosphoric_Acid_Mediated_Proton_Conductivit y_as_Fuel_Cell_Electrolytes.pdf
DOIs:
10.1002/macp.201600059
Source: PublicationPreSubmission
Source-ID: 123396227
Publication: Research - peer-review › Journal article – Annual report year: 2016
Ammonia oxidation at high pressure and intermediate temperatures

Ammonia oxidation experiments were conducted at high pressure (30 bar and 100 bar) under oxidizing and stoichiometric conditions, respectively, and temperatures ranging from 450 to 925 K. The oxidation of ammonia was slow under stoichiometric conditions in the temperature range investigated. Under oxidizing conditions the onset temperature for reaction was 850–875 K at 30 bar, while at 100 bar it was about 800 K, with complete consumption of NH₃ at 875 K. The products of reaction were N₂ and N₂O, while NO and NO₂ concentrations were below the detection limit even under oxidizing conditions. The data were interpreted in terms of a detailed chemical kinetic model. The rate constant for the reaction of the important intermediate H₂NO with O₂ was determined from ab initio calculations to be 2.3 × 10⁻⁸ T⁻².994 exp (−9510 K/T) cm³ mol⁻¹ s⁻¹. The agreement between experimental results and model work was satisfactory. The main oxidation path for NH₃ at high pressure under oxidizing conditions is NH₃ + OH → NH₂ + HO₂

NO + NH₂ → N₂ + OH, which promote the ammonia consumption by forming OH radicals, and to NH₂ + NO = N₂ + H₂O and NH₂ + NO₂ = N₂O + H₂O, which are the main chain-terminating steps.

General information

State: Published
Organizations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Technical University of Denmark, Wuhan University, University of North Texas
Authors: Song, Y. (Ekstern), Hashemi, H. (Intern), Christensen, J. M. (Intern), Zou, C. (Ekstern), Marshall, P. (Ekstern), Glarborg, P. (Intern)
Pages: 358–365
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Main Research Area: Technical/natural sciences

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Journal: Fuel
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ISSN (Print): 0016-2361
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.9 SJR 1.744 SNIP 2.179
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.809 SNIP 2.125 CiteScore 4.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.667 SNIP 2.331 CiteScore 4.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.811 SNIP 2.595 CiteScore 4.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.852 SNIP 2.465 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.093 SNIP 2.427 CiteScore 4.1
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.984 SNIP 2.319
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.012 SNIP 2.277
Amphiphilic copolymers for fouling-release coatings

Polydimethylsiloxane (PDMS) resins are extensively used as binder in fouling-release coatings due to the low critical surface energy and low elastic modulus of PDMS. These properties result in poor adhesion of the fouling organisms, which are therefore detached by hydrodynamic forces during navigation [1,2,3]. Other compounds are usually mixed together with the binder (e.g. silica and pigments) in order to improve the mechanical, thixotropic and visual properties of the coatings. It has been shown, however, that these ingredients have a negative effect on the fouling-release properties of the coatings [1,2,4].

Together with the PDMS-system, non-reactive polymers have been used to improve the fouling-release properties of the coatings. Initially, hydrophobic siloxane-based polymers were used, which aimed to increase the hydrophobicity of the PDMS surface [5,6]. However, copolymers comprising hydrophilic, amphiphilic and zwitterionic chemistries have been recently introduced due to their resistance to protein adsorption [7,8]. As a result, most of the current commercial fouling-release coatings contain either amphiphilic or hydrophilic copolymers to improve the fouling release properties of the coatings [9,10,11].

This work shows the effect of an amphiphilic copolymer that induces hydrophilicity on the surface of the silicone-based fouling release coatings. The behaviour of these copolymers within the coating upon immersion and the interaction of these surface-active additives with other compounds of the coatings are addressed.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Danish Polymer Centre, Hempel A/S
Authors: Noguer, A. C. (Intern), Olsen, S. M. (Ekstern), Hvilsted, S. (Intern), Kiil, S. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 18th International Congress on Marine Corrosion and Fouling, Toulon, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Albert_Camos_Noguer_abstract_2016.pdf
Source: PublicationPreSubmission
Source-ID: 127357722
Publication: Research - peer-review > Conference abstract for conference – Annual report year: 2016

A multiple length scale description of the mechanism of elastomer stretching

Conventionally, the stretching of rubber is modeled exclusively by rotations of segments of the embedded polymer chains; i.e. changes in entropy. However models have not been tested on all relevant length scales due to a lack of appropriate
probes. Here we present a universal X-ray based method for providing data on the structure of rubbers in the 2-50 angstrom range. First results relate to the elongation of a silicone rubber. We identify several non-entropic contributions to the free energy and describe the associated structural changes. By far the largest contribution comes from structural changes within the individual monomers, but among the contributions is also an elastic strain, acting between chains, which is 3-4 orders of magnitude smaller than the macroscopic strain, and of the opposite sign, i.e. extension of polymer chains in the direction perpendicular to the stretch. This may be due to trapped entanglements relaxing to positions close to the covalent crosslinks.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Physics, Neutrons and X-rays for Materials Physics, Oak Ridge National Laboratory, University of New South Wales, European Synchrotron Radiation Facility, Roskilde University
Authors: Neuefeind, J. (Ekstern), Skov, A. L. (Intern), Daniels, J. E. (Ekstern), Honkimaki, V. (Ekstern), Jakobsen, B. (Ekstern), Oddershede, J. (Intern), Poulsen, H. F. (Intern)
Pages: 95910-95919
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: RSC Advances
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Issue number: 98
ISSN (Print): 2046-2069
Ratings:
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Original language: English
Electronic versions:
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DOI:
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Source-ID: 2346514394
Publication: Research - peer-review › Journal article – Annual report year: 2016

Anaerobic co-digestion of perennials: Methane potential and digestate nitrogen fertilizer value: Methane potential and digestate nitrogen fertilizer value
Co-digestion of crop biomass improves the traditional manure-based biogas yield due to an increased content of easily degradable carbon compounds. In this study, the methane potential of three perennials (grass, legumes, and
grass+legume) was determined using various amounts together with animal manure. The nitrogen (N) mineralization
dynamics in soil and the N-fertilizer value of the derived digestates were subsequently tested in both a soil incubation
study and a pot experiment with spring barley. Digestion of all tested perennials together with a manure-based inoculum
increased the cumulative methane yield four to five times compared to digestion of the inoculum alone, with the highest
increases observed with pure grass. However, the methane potential decreased along with increasing grass biomass
concentration. In the plant pot experiment, all tested digestates increased barley shoot biomass by 40-170%, to an extent
statistically comparable to mineral N fertilizer. However, the application of the digestate originating from fermentation with
pure grass resulted in lower plant growth and a more fluctuating soil mineral N content throughout the incubation study
compared to the other digestates. Considering the high dry matter and methane yield ha⁻¹, the possibility to substitute
mineral N fertilizer inputs by leguminous biological N₂ fixation capacity, and the digestate fertilizer value, the integration of
grass-legume mixtures or sole legumes into anaerobic digestion systems as co-substrate for manure seems to be
promising. This could furthermore contribute to the diversification of cropping systems for bioenergy production.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, University of
Copenhagen, Suez Environnement, Roskilde University
Authors: Muller-Stover, D. S. (Ekstern), Sun, G. (Intern), Kroff, P. (Ekstern), Thomsen, S. T. (Ekstern), Hauggaard-
Nielsen, H. (Ekstern)
Pages: 696-704
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.15 SJR 0.813 SNIP 1.131
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.825 SNIP 0.954 CiteScore 2.02
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.717 SNIP 1.199 CiteScore 1.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.844 SNIP 1.149 CiteScore 1.94
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.853 SNIP 1.274 CiteScore 1.74
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.205 SNIP 1.318 CiteScore 2.19
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.937 SNIP 0.99
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.991 SNIP 0.978
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.849 SNIP 0.992
Scopus rating (2007): SJR 0.743 SNIP 0.95
Scopus rating (2006): SJR 0.7 SNIP 0.862
Scopus rating (2005): SJR 0.849 SNIP 0.869
Analysis and modeling of alkali halide aqueous solutions

A new model is proposed for correlation and prediction of thermodynamic properties of electrolyte solutions. In the proposed model, terms of a second virial coefficient-type and of a KT-UNIFAC model are used to account for a contribution of binary interactions between ion and ion, and water and ion, respectively, with a Debye-Hückel term for electrostatic interactions. In a second approach of the model, additional parameters for interactions of ion pairs in the KT-UNIFAC are introduced as a correction to get better agreement with data. Structural parameters of ions used in the framework of UNIFAC or UNIQUAC are newly estimated using ionic radii for physically correct representation of the combinatorial part. Including temperature-dependent coefficients in the interaction parameters, significant improvements in accuracy are achieved for a wide range of temperatures. This work is focused on calculations for various electrolyte properties of alkali halide aqueous solutions such as mean ionic activity coefficients, osmotic coefficients, and salt solubilities. The model covers highly nonideal electrolyte systems such as lithium chloride, lithium bromide and lithium iodide, that is, systems that are very soluble in water, for example, up to more than 30 mol kg\(^{-1}\). Phase behaviors for the systems are analyzed at concentrations of salt up to the solubility in water at temperatures between 273 and 373 K by comparing calculated results with available experimental data and available models.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Korea University
Authors: Kim, S. H. (Ekstern), Anantpinijwatna, A. (Intern), Kang, J. W. (Ekstern), Gani, R. (Intern)
Pages: 177-198
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Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 412
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
An efficient arabinoxylan-debranching α-l-arabinofuranosidase of family GH62 from Aspergillus nidulans contains a secondary carbohydrate binding site

An α-l-arabinofuranosidase of GH62 from Aspergillus nidulans FGSC A4 (AnAbf62A-m2,3) has an unusually high activity towards wheat arabinoxylan (WAX) (67 U/mg; $k_{\text{cat}} = 178/s$, $K_{\text{m}} = 4.90 \text{ mg/ml}$) and arabinoxylooligosaccharides (AXOS) with degrees of polymerisation (DP) 3–5 (37–80 U/mg), but about 50 times lower activity for sugar beet arabinan and 4-nitrophenyl-α-l-arabinofuranoside. α-1,2- and α-1,3-linked arabinofuranoses are released from monosubstituted, but not from disubstituted, xylose in WAX and different AXOS as demonstrated by NMR and polysaccharide analysis by carbohydrate gel electrophoresis (PACE). Mutants of the predicted general acid (Glu188) and base (Asp28) catalysts, and the general acid pKa modulator (Asp136) lost 1700-, 165- and 130-fold activities for WAX. WAX, oat spelt xylan, birchwood xylan and barley β-glucan retarded migration of AnAbf62A-m2,3 in affinity electrophoresis (AE) although the latter two are neither substrates nor inhibitors. Trp23 and Tyr44, situated about 30 Å from the catalytic site as seen in an AnAbf62A-m2,3 homology model generated using Streptomyces thermoviolaceus SthAbf62A as template, participate in carbohydrate binding. Compared to wild-type, W23A and W23A/Y44A mutants are less retarded in AE, maintain about 70 % activity towards WAX with $K_i$ of WAX substrate inhibition increasing 4–7-folds, but lost 77–96 % activity for the AXOS. The Y44A single mutant had less effect, suggesting Trp23 is a key determinant. AnAbf62A-m2,3 seems to apply different polysaccharide-dependent binding modes, and Trp23 and Tyr44 belong to a putative surface binding site which is situated...
at a distance of the active site and has to be occupied to achieve full activity.

**General information**

State: Published

Organisations: Department of Systems Biology, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Enzyme and Protein Chemistry, Department of Chemistry, Metalloprotein Chemistry and Engineering, Organic Chemistry, Carlsberg Laboratory, University of Cambridge, University of Copenhagen, Megazyme International Ireland Ltd.


Number of pages: 13
Pages: 6265-6277
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Main Research Area: Technical/natural sciences

**Publication information**

Journal: Applied Microbiology and Biotechnology
Volume: 100
Issue number: 14
ISSN (Print): 0175-7598
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.57 SJR 1.177 SNIP 1.173
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.254 SNIP 1.217 CiteScore 3.43
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.327 SNIP 1.458 CiteScore 3.71
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.533 SNIP 1.432 CiteScore 4.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.507 SNIP 1.286 CiteScore 4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.437 SNIP 1.232 CiteScore 3.72
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.381 SNIP 1.239
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.353 SNIP 1.062
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.224 SNIP 0.979
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.036 SNIP 1.021
A new look at extensional rheology of low-density polyethylene

The nonlinear rheology of three selected commercial low-density polyethylenes (LDPE) is measured in uniaxial extensional flow. The measurements are performed using three different devices including an extensional viscosity fixture (EVF), a homemade filament stretching rheometer (DTU-FSR) and a commercial filament stretching rheometer (VADER-1000). We show that the measurements from the EVF are limited by a maximum Hencky strain of 4, while the two filament stretching rheometers are able to probe the nonlinear behavior at larger Hencky strain values where the steady state is reached. With the capability of the filament stretching rheometers, we show that LDPEs with quite different linear viscoelastic properties can have very similar steady extensional viscosity. This points to the potential for independently controlling shear and extensional rheology in certain rate ranges.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Dow Benelux B.V., Drexel University, Dow Chemical Company
Authors: Huang, Q. (Intern), Mangnus, M. (Ekstern), Alvarez, N. J. (Ekstern), Koopmans, R. (Ekstern), Hassager, O. (Intern)
Pages: 343-350
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Rheologica Acta
Volume: 55
Issue number: 5
ISSN (Print): 0035-4511
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.9 SJR 0.61 SNIP 1.035
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Gas-solid systems are applied in various industries such as pharmaceutical, food industry and chemical processes like catalytic cracking, combustion and gasification. One of the leading technologies to deal with such processes is the fluidized bed technology. Considering the increasing demands on production, process and application of solid particles, investigation, characterization and optimization of the whole or a part of a fluidized bed system is getting vital. Nowadays, fine particles are utilized in lots of number of applications and due to present challenges in fluidization of these type of particles, assistive methods are applied to make it possible. One the major points where these challenges impacts is the loop-seals. Conventional loop-seal are operated around minimum fluidization condition and definitely fine particles has difficulties to be operated under this regime. The goal of the thesis is to design a new version of a non-mechanical valve for transportation of the particles and closing the loop in circulating or interconnected fluidized bed systems. As the
primary proposal, combination of three assistive methods (tapered fluidized bed, mixture of coarse and fine particles and high velocity gas jet) in a single device was examined to check feasibility of handling the fine particles. A draft tube spouted bed is considered to be operated with coarse particles and the standpipe which is filled with fine particles represents the downcomer of an acyclone. This set-up was somewhat capable of transporting the fine particles but introducing the particles through an inclined tube was not possible. After performing some supportive experiments, new version of the experimental set-up, namely four draft tubes pneumatic transport (4-DTPT), was design, constructed and examined. Successful introduction and transportation of fine particles are observed for this device. For the purpose of characterization of the 4-DTPT test rig, different type of experiments were performed considering changes in operating conditions and geometric parameters as well as the particles size. Although, more investigations are needed to be carried out to thoroughly characterize and optimize the new device. Further analysis, modifications, corrections and systematic investigation of the 4-DTPT will provide the knowledge about scale-up of this device to be utilized for industrial applications.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Azizaddini, S. (Intern), Dam-Johansen, K. (Intern), Lin, W. (Intern)
Number of pages: 146
Publication date: 2016

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Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
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**Bibliographical note**
"This thesis was presented publicly first in the defense session (28th April 2016) and published in June 2016"

**Relations**
Projects:
A New Type of Non-Mechanical Valves for Recirculation of Fine Particles
Publication: Research › Ph.D. thesis – Annual report year: 2016

**An Experimental and Theoretical Study of CO2 Hydrate Formation Systems**
Hydrate crystallization can become equally important carbon capture method provided that this technology undergoes further research. Toward this objective, this study tries to shed light on a quite new topic of research: hydrate promotion. Hydrate promotion implies the production of hydrate at lower pressures (and thus lower adjunctive capital/operational costs) by the use of special chemicals (promoters).
At first, extensive literature review has shown that both experimental data and modeling in this subject are imperative. Therefore, experimental data were produced and published (see Appendix E) using as promoters tetra-n-butyl ammonium salts of bromide, fluoride and cyclopentane in collaboration with MINESParisTech in France. These chemicals are well known for their reduction capabilities of hydrate formation pressure. The results are in good accordance with the literature. Moreover, the simultaneous combination of these chemicals achieved greater pressure reduction than if they were used separately. Then, experimental uncertainties were measured (for pressure/temperature transducers and gas chromatograph) and calculated (for the inserted quantities of water and chemicals). The uncertainties were at an acceptable level for all cases. A further evaluation of the experimental data, regarding their consistency, included the use of Clapeyron equation. It was shown that the results of this work and many of the systems from literature are quite satisfactory. Finally, the well-known van der Waals-Platteeuw hydrate model coupled with CPA EoS was used against experimental data as it was developed in CERE, DTU. The model predicted very satisfactory the CP results of this work and also other CO2+cyclolkane hydrate results from literature. This model’s consistency lies inter alia on the ground that fluid phases were modeled only with CPA EoS while correlations are utilized in current publications for the aqueous phase and an EoS for the hydrate phase.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, KT Consortium, MINES ParisTech
Authors: Tzirakis, F. (Intern), Kontogeorgis, G. (Intern), Coquelet, C. (Ekstern), von Solms, N. (Intern), Stringari, P. (Ekstern)
Number of pages: 146
Publication date: 2016

**Publication information**
Hydrogen sulfide oxidation experiments were conducted in \( \text{O}_2/\text{N}_2 \) at high pressure (30 and 100 bar) under oxidizing and stoichiometric conditions. Temperatures ranged from 450 to 925 K, with residence times of 3–20 s. Under stoichiometric conditions, the oxidation of H\(_2\)S was initiated at 600 K and almost completed at 900 K. Under oxidizing conditions, the onset temperature for reaction was 500–550 K, depending on pressure and residence time, with full oxidization to SO\(_2\) at 550–600 K. Similar results were obtained in quartz and alumina tubes, indicating little influence of surface chemistry. The data were interpreted in terms of a detailed chemical kinetic model. The rate constants for selected reactions, including \( \text{SH} + \text{O}_2 \rightarrow \text{SO}_2 + \text{H} \), were determined from ab initio calculations. Modeling predictions generally overpredicted the temperature for onset of reaction. Calculations were sensitive to reactions of the comparatively unreactive SH radical. Under stoichiometric conditions, the oxidation rate was mostly controlled by the \( \text{SH} + \text{SH} \) branching ratio to form H\(_2\)S + S (promoting reaction) and HSSH (terminating). Further work is desirable on the \( \text{SH} + \text{SH} \) recombination and on subsequent reactions in the S\(_2\) subset of the mechanism. Under oxidizing conditions, a high \( \text{O}_2 \) concentration (augmented by the high pressure) causes the termolecular reaction \( \text{SH} + \text{O}_2 + \text{O}_2 \rightarrow \text{HSO} + \text{O}_3 \) to become the major consumption step for SH, according to the model. Consequently, calculations become very sensitive to the rate constant and product channels for the H\(_2\)S + \( \text{O}_3 \) reaction, which are currently not well established.
An Aspergillus nidulans GH26 endo-β-mannanase with a novel degradation pattern on highly substituted galactomannans

The activity and substrate degradation pattern of a novel Aspergillus nidulans GH26 endo-β-mannanase (AnMan26A) was investigated using two galactomannan substrates with varying amounts of galactopyranosyl residues. The AnMan26A was characterized in parallel with the GH26 endomannanase from Podospora anserina (PaMan26A) and three GH5 endomannanases from A. nidulans and Trichoderma reesei (AnMan5A, AnMan5C and TrMan5A). The initial rates and the maximal degree of enzymatically catalyzed conversion of locust bean gum and guar gum galactomannans were determined. The hydrolysis product profile at maximal degree of conversion was determined using DNA sequencer-Assisted Saccharide analysis in High throughput (DASH). This is the first reported use of this method for analyzing galactomannooligosaccharides. AnMan26A and PaMan26A were found to have a novel substrate degradation pattern on the two galactomannan substrates. On the highly substituted guar gum AnMan26A and PaMan26A reached 35-40% as their maximal degree of conversion whereas the three tested GH5 endomannanases only reached 8-10% as their maximal degree of conversion. α-Galactosyl-mannose was identified as the dominant degradation product resulting from AnMan26A and PaMan26A action on guar gum, strongly indicating that these two enzymes can accommodate galactopyranosyl residues in the -1 and in the +1 subsite. The degradation of α-64-63-di-galactosyl-mannopentaose by AnMan26A revealed accommodation of galactopyranosyl residues in the -2, -1 and +1 subsite of the enzyme. Accommodation of galactopyranosyl residues in subsites -2 and +1 has not been observed for other characterized endomannanases to date. Docking analysis of galactomannooligosaccharides in available crystal structures and homology models supported the conclusions drawn from the experimental results. This newly discovered diversity of substrate degradation patterns demonstrates an expanded functionality of fungal endomannanases, than hitherto reported.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Novozymes A/S, Lund University
An integrated knowledge-based and optimization tool for the sustainable selection of wastewater treatment process concepts

The increasing demand on wastewater treatment plants (WWTPs) has involved an interest in improving the alternative treatment selection process. In this study, an integrated framework including an intelligent knowledge-based system and superstructure-based optimization has been developed and applied to a real case study. Hence, a multi-criteria analysis together with mathematical models is applied to generate a ranked short-list of feasible treatments for three different scenarios. Finally, the uncertainty analysis performed allows for increasing the quality and robustness of the decisions considering variation in influent concentrations. For the case study application, the expert system identifies 5 potential process technologies and, using this input, the superstructure identifies membrane bioreactors as the optimal and robust solution under influent uncertainties and tighter effluent limits. A mutual benefit and synergy is achieved when both tools are integrated because expert knowledge and expertise are considered together with mathematical models to select the most appropriate treatment alternative.
A novel analytical method for D-glucosamine quantification and its application in the analysis of chitosan degradation by a minimal enzyme cocktail

Enzymatic depolymerization of chitosan, a β-(1,4)-linked polycationic polysaccharide composed of D-glucosamine (GlcN) and N-acetyl-D-glucosamine (GlcNAc) provides a possible route to the exploitation of chitin-rich biomass. Complete conversion of chitosan to mono-sugars requires the synergistic action of endo- and exo- chitosanases. In the present study we have developed an efficient and cost-effective chitosan-degrading enzyme cocktail containing only two enzymes, an endo-attacking bacterial chitosanase, ScCsn46A, from *Streptomyces coelicolor*, and an exo-attacking glucosamine specific β-glucosaminidase, Tk-Glm, from the archaeon *Thermococcus kodakarensis* KOD1. Moreover, we developed a fast, reliable quantitative method for analysis of GlcN using high performance anion exchange chromatography with pulsed amperometric detection (HPAEC-PAD). The sensitivity of this method is high and less than 50 pmol was easily detected, which is about 1000-fold better than the sensitivity of more commonly used detection methods based on refractive index. We also obtained qualitative insight into product development during the enzymatic degradation reaction by means of ElectroSpray Ionization-Mass Spectrometry (ESI-MS).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Norwegian University of Life Sciences, Apronex s.r.o., Biotech Surindo
Pages: 18-24
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Application of a systematic methodology for sustainable carbon dioxide utilization process design

As concerns about the environment are growing, new efforts are needed to achieve more sustainable processes. One such environmental concern is global warming, which is primarily caused by the greenhouse effect or the increase in concentration of greenhouse gases [1]. The most significant greenhouse gases are carbon dioxide, methane and nitrous oxide, of which carbon dioxide is the highest constituent at 82%. Furthermore, the amount of carbon dioxide emissions is growing with time. These trends make it evident that there is a need for methods to reduce these greenhouse gases emissions. While there are two methods of reducing carbon dioxide emissions, carbon capture and storage (CCS) and carbon capture and utilization (CCU), CCU is considered promising as it makes further use of the carbon dioxide as a solvent, raw material, and reagent to produce valuable products [1]. Using such utilization processes, the emissions can be reduced as they are being utilized and profit can be obtained, or the cost of operation for the carbon dioxide treatment can be returned, through this utilization process.

In order to systematically reduce such emissions, carbon capture and utilization is considered rather than carbon capture and storage. To achieve this a methodology is developed to design sustainable carbon dioxide utilization processes. First, the information on the possible utilization alternatives is collected, including the economic potential of the process and the carbon dioxide emissions. The carbon dioxide emissions can be classified as direct and indirect emissions in a chemical process. The net carbon dioxide is determined for the utilization processes as the indirect carbon dioxide emissions minus the carbon dioxide utilized. Processes that present zero or negative net carbon dioxide emission are desired in order to reduce the carbon dioxide emissions. Using this estimated preliminary evaluation, the top processes, with the most negative carbon dioxide emission are investigated by rigorous detailed simulation to evaluate the net carbon dioxide emissions. Once the base case design is established and evaluated, targeted improvements are made by exploiting opportunities, for example, optimization, heat integration and improved design decisions so that more sustainable and lower net carbon dioxide emission alternatives are obtained.

This method is applied to various processes where carbon dioxide is used as raw material. First, the process data are collected and compared. The economic feasibility is evaluated. From this, five processes are selected and analyzed in detail: the production of dimethyl carbonate, succinic acid, propylene carbonate, dimethyl ethylene and methanol. Not all the studied processes could be designed for zero or negative net carbon dioxide emission. Propylene carbonate production is found to have a negative net carbon dioxide, where, implementing targeted process improvements minimized the net carbon dioxide emission to -0.389 kg of carbon dioxide per kg of propylene carbonate. On the other hand, for succinic acid production, even after targeted improvements, the net carbon dioxide remained positive, even though compared to the existing industrial processes there is a relative reduction of up to 85%.

What this study shows is that for meaningful net carbon dioxide reduction, the carbon dioxide utilization processes need to be selected very carefully to obtain the best results. However, the opportunity to potentially reduce the net carbon dioxide emissions for the production of some bulk chemicals with carbon dioxide as feedstock exists.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, Technical University of Denmark
Authors: Plaza, C. C. (Ekstern), Frauzem, R. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Abstract_2016_no_2.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Application of e-KT-UNIFAC Model for Improved and Innovative Design of Biphasic Reacting Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana, Korea University
Authors: Anantpinijwatna, A. (Intern), Hyung Kim, S. (Ekstern), Sales-Cruz, M. (Ekstern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2016
Application of NAD(P)H oxidase for cofactor regeneration in dehydrogenase catalyzed oxidations

Biocatalytic oxidations can offer clear advantages compared to chemically catalyzed oxidations in terms of chemo, regio and stereoselectivity as well as a reduced environmental impact. One of the most industrially important reactions is the oxidation of alcohols, which can be carried out using alcohol dehydrogenases. However, their effective use requires an effective regeneration of the oxidized nicotinamide cofactor (NAD(P)⁺), which is critical for the economic feasibility of the process. NAD(P)H oxidase is an enzyme class of particular interest for this cofactor regeneration since it enables the use of molecular oxygen as a substrate, generating either water or hydrogen peroxide as a by-product. The use of these enzymes is now gaining an increased interest, and several different enzymes of both types have been applied for proof-of-concept. In this review, we give an overview of the state-of-the-art, and discuss several important issues for future implementation in a production process.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Rehn, G. (Intern), Pedersen, A. T. (Intern), Woodley, J. (Intern)
Pages: 331–339
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Molecular Catalysis B: Enzymatic
Volume: 134
Issue number: Part B
ISSN (Print): 1381-1177
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.63 SNIP 0.855
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.66 SNIP 0.802 CiteScore 2.12
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.744 SNIP 1.044 CiteScore 2.5
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.038 SNIP 1.38 CiteScore 3.09
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.12 SNIP 1.347 CiteScore 2.98
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.026 SNIP 1.126 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.797 SNIP 1.032
BFI (2009): BFI-level 1
Application of the e-KT-UNIFAC Model for the Improved and Innovative Design of Biphasic Reacting Systems

Biphasic reacting systems contain effectively immiscible aqueous and organic liquid phases in which reactants, products, and catalysts can partition. These conditions allow novel synthesis paths, higher yields, and faster reactions, as well as facilitate product(s) separation. A systematic modeling framework of three modules has been developed to describe phase equilibria, reactions, mass transfer, and material balances of such processes. The recently developed group-contribution electrolyte model, e-KT-UNIFAC, is used to predict the-partitioning and equilibria of electrolyte and nonelectrolyte species for a wide variety of reacting substances. Reaction kinetics and mass transfer are described by nonelementary reaction rate laws. Extents of reaction are used to calculate the species material balances. The resulting mathematical model contains only a few rate parameters to be regressed to a minimum of time-dependent data. In addition to describing the behavior of such systems, predictions can be made of the effectiveness in rates and ultimate amounts of product formation using different organic solvents. The present paper briefly describes the framework and applies it to the cases of epoxidation of palm oil and production of furan derivatives.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, Korea Advanced Institute of Science & Technology, Universidad Autonoma Metropolitana, University of Virginia
Authors: Anantpinijwatna, A. (Intern), Kim, S. H. (Ekstern), Sales-Cruz, M. (Ekstern), O'Connell, J. P. (Ekstern), Gani, R. (Intern)
Pages: 4090-4103
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical & Engineering Data
Volume: 61
Issue number: 12
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Application of various water soluble polymers in gas hydrate inhibition

Formation of hydrates in gas transmission lines due to high pressures and low temperatures is a serious problem in the oil and gas industry with potential hazards and/or economic losses. Kinetic hydrate inhibitors are water soluble polymeric compounds that prevent or delay hydrate formation. This review presents the various types of water soluble polymers used for hydrate inhibition, including conventional and novel polymeric inhibitors along with their limitations. The review covers the relevant properties of vinyl lactam, amide, dendrimeric, fluorinated, and natural biodegradable polymers.
factors affecting the performance of these polymers and the structure-property relationships are reviewed. A comprehensive review of the techniques used to evaluate the performance of the polymeric inhibitors is given. This review also addresses recent developments, current and future challenges, and field applications of a range of polymeric kinetic hydrate inhibitors.

**General information**

**State:** Published  
**Organisations:** Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, King Fahd University of Petroleum and Minerals, Qatar University  
**Authors:** Kamal, M. S. (Ekstern), Hussein, I. A. (Ekstern), Sultan, A. S. (Ekstern), von Solms, N. (Intern)  
**Pages:** 206-225  
**Publication date:** 2016  
**Main Research Area:** Technical/natural sciences

**Publication information**

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**Volume:** 60  
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**Ratings:**  
BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 9.52 SJR 3.051 SNIP 3.454  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 2.999 SNIP 3.387 CiteScore 8.35  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 3.106 SNIP 3.761 CiteScore 7.79  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 3.072 SNIP 3.889 CiteScore 7.88  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 2.814 SNIP 3.915 CiteScore 7.24  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 2.787 SNIP 3.901 CiteScore 7.39  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 2.374 SNIP 3.112  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 2.494 SNIP 3.6  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 2.447 SNIP 3.127  
Web of Science (2008): Indexed yes  
Scopus rating (2006): SJR 0.889 SNIP 1.758  
Scopus rating (2005): SJR 0.956 SNIP 2.649  
Scopus rating (2004): SJR 1.152 SNIP 2.268  
Scopus rating (2003): SJR 0.813 SNIP 2.492
A Rapid Selection Procedure for Simple Commercial Implementation of omega-Transaminase Reactions

A stepwise selection procedure is presented to quickly evaluate whether a given omega-transaminase reaction is suitable for a so-called "simple" scale-up for fast industrial implementation. Here "simple" is defined as a system without the need for extensive process development or specialized equipment. The procedure may be used when investment in intensive process development cannot be justified or when rapid execution is paramount, for applications such as small singular batches. The three step evaluation procedure consists of: (1) thermodynamic assessment, (2) biocatalyst activity screening, and (3) determination of product inhibition. The method is exemplified with experimental work focused on two products: 1-(4-bromophenyl)ethylamine and (S)-(+)3-amino-1-Boc-piperidine, synthesized from their corresponding pro-chiral ketones each with two alternative amine donors, propan-2-amine, and 1-phenylethylamine. Each step of the method has a threshold value, which must be surpassed to allow "simple" implementation, helping select suitable combinations of substrates, enzymes, and donors. One reaction pair, 1-Boc-3-piperidone with propan-2-amine, met the criteria of the three-step selection procedure and was subsequently run at 25 mL scale synthesizing (S)-(+)3-amino-1-Boc-piperidine at concentrations up to 75 g/L. However, the highest product yield (70%) was obtained at a lower substrate concentration of 50 g/L.
A replicated climate change field experiment reveals rapid evolutionary response in an ecologically important soil invertebrate

Whether species can respond evolutionarily to current climate change is crucial for the persistence of many species. Yet, very few studies have examined genetic responses to climate change in manipulated experiments carried out in natural field conditions. We examined the evolutionary response to climate change in a common annelid worm using a controlled replicated experiment where climatic conditions were manipulated in a natural setting. Analyzing the transcribed genome of 15 local populations, we found that about 12% of the genetic polymorphisms exhibit differences in allele frequencies associated to changes in soil temperature and soil moisture. This shows an evolutionary response to realistic climate change happening over short-time scale, and calls for incorporating evolution into models predicting future response of species to climate change. It also shows that designed climate change experiments coupled with genome sequencing offer great potential to test for the occurrence (or lack) of an evolutionary response.
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<td>SJR 2.715 SNIP 1.48</td>
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A review: Fly ash and deposit formation in PF fired biomass boilers

In recent years suspension fired boilers have been increasingly used for biomass based heat and power production in several countries. This has included co-firing of coal and straw, up to 100% firing of wood or straw and the use of additives to remedy problems with biomass firing. In parallel to the commercialization of the suspension biomass firing technology a range of research studies have improved our understanding of the formation of fly ash and the impact on deposit formation and corrosion in such boilers. In this paper a review of the present knowledge with respect to ash and deposit formation in biomass suspension fired boilers is provided. Furthermore the influence of co-firing and use of additives on ash chemistry, deposit properties and boiler operation is discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Jensen, P. A. (Intern), Jappe Frandsen, F. (Intern), Wu, H. (Intern), Glarborg, P. (Intern)
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Biomass, Suspension firing, Deposits, Ash
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1601_A_review._Fly_ash_and_deposit_formation_in_PF_fired_biomass_boilers.pdf
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Ash behavior and de-fluidization in low temperature circulating fluidized bed biomass gasifier

Biomass is increasingly used as a fuel for power generation. Herbaceous fuels however, contain high amounts of alkali metals which get volatilized at high temperatures and forms salts with low melting points and thus condense on pipelines, reactor surfaces and may cause de-fluidization. A Low-Temperature Circulating Fluidized Bed System (LTCFB) gasifier allows pyrolysis and gasification of biomass to occur at low temperatures thereby improving the retention of alkali and other ash species within the system and minimizing the amount of ash species in the product gas. In addition, the low reactor temperature ensures that high-alkali biomass fuels can be used without risks of bed de-fluidization. This thesis aims to understand the behavior of alkali metals and ash in the LTCFB system. The thesis work involved measurements made on bed material and product gas dust samples on a 100kW LTCFB gasifier placed at Risø and a 6 MW LTCFB gasifier owned by DONG ENERGY and placed in Kalundborg. In addition to the analysis of the inorganic elemental composition of the collected samples, SEM and TGA analysis of the samples were made to improve understanding on the behavior of the ash forming species within the system. It was observed that of the total fuel ash entering the system, a large fraction (40-50%) of the ash was retained in the secondary cyclone bottoms and a lower amount (8-10%) was released as dust in the exit gas; the residual ash was accumulated within the fluidized bed system. A dominant fraction of alkali and alkaline earth metals were retained in condensed state along with Si and some Cl, while a large fraction of Cl and S appeared in gaseous form and was released with the product gas. Measurements on the product gas from the 100 kW LTCFB gasifier showed the presence of Cl in the form of gaseous methyl chlorides (90-100 ppm). Release of K and other inorganic species with the tar in the product gas from the LTCFB gasifier were found to be low. The major forms in which K and Si could exist in the LTCFB gasifier are K-salts (KCl and K2CO3), organically bound K (K bound to ion exchange sites of the char matrix and intercalated K), and K-silicates. At the temperature in the pyrolysis chamber (6500C) of the LTCFB gasifier, the above K species are expected to be mostly present in the solid state. In the char reactor (where the char from the pyrolysis chamber is gasified and combusted at temperatures around 7300C), KCl(s) will partially vaporize and the released K could react with silica to form silicates. When the flue gas enters the pyrolysis reactor, the temperature is reduced and KCl aerosols are formed. The release and retention of the condensed ash species from the system was seen to be controlled by the ash particle size and the cut size of the primary and secondary cyclones. A model accounting for the ash collection by the plant cyclones was developed which predicted the product gas ash particle release reasonably well.
The present work also aims to understand the effect of biomass fuel ash composition and fluid bed operation conditions especially temperature on agglomeration and de-fluidization of alkali-rich bed material under gasification conditions. The de-fluidization studies involved measurements with mixtures of sand and pure potassium salts (KCl and K2CO3) as well as bed material samples obtained from a 6 MW Low Temperature Circulating Fluidized bed (LTCFB) gasifier on a bench-scale fluidized bed reactor set up. The mechanism of agglomeration in the bed particles was seen to vary with the speciation of K. It was seen that in sand and KCl agglomerates, the sand particles were bound by KCl melts. There was very limited chemical reaction observed between KCl and the sand particles with no presence of silicate melts in the agglomerates. In sand and K2CO3 mixtures and the LT-CFB bed material samples the agglomeration was seen to occur due to a coating of viscous silicate melts formed from reaction of alkaline and alkali earth species with silica from the bed particles (coating induced agglomeration). It was also seen that the composition of the bed particles affected the de-fluidization temperatures. The de-fluidization took place at higher temperatures in the case of LTCFB bed material particles (780-7850°C) as compared to the sand and K2CO3 mixtures (7300°C) with similar K contents (4.2-4.5%), though both showed that the de-fluidization occurred by the mechanism of coating induced agglomeration. This is attributed to the presence of Ca and Mg in the bed particles; these elements shift the formation of the eutectic melts to higher temperatures increasing the viscosity levels of the coatings. A mathematical model for de-fluidization of alkali rich bed material was developed to predict the de-fluidization temperatures as a function of parameters such as initial alkali concentrations within the bed particle diameters and the fraction of K entrained from the system. The model was also applied to study the de-fluidization behavior of alkali-rich samples in a large scale LTCFB gasifier. The model was used to predict the variations in de-fluidization time on a full scale LTCFB plant with respect to parameters such as temperature, fuel alkali concentrations and bed particle diameter.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Narayan, V. (Intern), Glarborg, P. (Intern), Jensen, P. A. (Intern), Henriksen, U. B. (Intern)
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Publication date: 2016

A simple method for reducing inevitable dielectric loss in high-permittivity dielectric elastomers
Commercial viability of dielectric elastomers (DEs) is currently limited by a few obstacles, including high driving voltages (in the kV range). Driving voltage can be lowered by either decreasing the Young's modulus or increasing the dielectric permittivity of silicone elastomers, or a combination thereof. A decrease in the Young’s modulus, however, is often accompanied by a loss in mechanical stability, whereas increases in dielectric permittivity are usually followed by a large increase in dielectric loss followed by a decrease in breakdown strength and thereby the lifetime of the DE. A new soft elastomer matrix, with high dielectric permittivity and a low Young's modulus, aligned with no loss of mechanical stability, was prepared through the use of commercially available chloropropyl-functional silicone oil mixed into a tough commercial liquid silicone rubber silicone elastomer. The addition of chloropropyl-functional silicone oil in concentrations up to 30 phr was found to improve the properties of the silicone elastomer significantly, as dielectric permittivity increased to 4.4, dielectric breakdown increased up to 25% and dielectric losses were reduced. The chloropropyl-functional silicone oil also decreased the dielectric losses of an elastomer containing dielectric permittivity-enhancing TiO2 fillers. Commercially available chloropropyl-functional silicone oil thus constitutes a facile method for improved silicone DEs, with very low dielectric losses.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Madsen, F. B. (Intern), Yu, L. (Intern), Mazurek, P. S. (Intern), Skov, A. L. (Intern)
Publication date: 2016
Main Research Area: Technical/natural sciences
A simple method for reducing inevitable dielectric loss in high permittivity dielectric elastomers.
A Solvent-Free Base Liberation of a Tertiary Aminoalkyl Halide by Flow Chemistry

A flow setup for base liberation of 3-(N,N-dimethylamino)propyl chloride hydrochloride and solvent-free separation of the resulting free base has been developed. Production in flow profits from an on-demand approach, useful for labile aminoalkyl halides. The requirement for obtaining a dry product has been fulfilled by the simple use of a saturated NaOH solution, followed by isolation of the liquid phases by gravimetric separation. The flow setup has an E factor reduction of nearly 50%, and a distillation step has been avoided. The method exemplifies how flow chemistry can be exploited to simplify, improve, and optimize manufacturing processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, H. Lundbeck A/S
Authors: Pedersen, M. J. (Intern), Skovby, T. (Eks), Mealy, M. J. (Eks), Dam-Johansen, K. (Intern), Kiil, S. (Intern)
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Scopus rating (2016): CiteScore 2.48 SJR 1.062 SNIP 0.859
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.318 SNIP 1.029 CiteScore 2.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 0.99 CiteScore 2.38
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.13 SNIP 0.977 CiteScore 2.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.185 SNIP 1.12 CiteScore 2.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.212 SNIP 0.914 CiteScore 2.22
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.114 SNIP 0.97
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.046 SNIP 0.922
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.943 SNIP 0.901
Assessing the environmental sustainability of early stage design for bioprocesses under uncertainties: An analysis of glycerol bioconversion

The development of a bio-based economy is seen as a key strategy towards a sustainable society in a world facing climate change, energy security and social distress. However, since substantial uncertainty is involved in early-stage design analyses, the ranking and identification of potential sustainable solutions is a challenging task. This work aims at facilitating the environmental sustainability assessment under uncertainty at the conceptual design of bioprocesses. This, in turn, enables screening design alternatives, and establishing a ranking of the most promising pathways. To this end, a step-wise methodology has been proposed to assist decision-makers to: (i) collect and generate the input data for bioprocesses; (ii) systematically reduce uncertainty concerning the material fluxes at the early stage design of bioprocesses, reducing overall uncertainty in the life cycle inventory; (iii) handle parameter uncertainty, by applying the Monte Carlo technique for the propagation of uncertainty in characterization factors to the potential impact categories’ outcomes; (iv) establish sound quantitative thresholds for alternatives comparison by incorporating a probabilistic interpretation; and lastly, (v) rank the alternatives within the design space. Finally, the methodology’s applicability is highlighted by screening early-stage glycerol bioconversion routes to value-added chemicals for future biorefinery concepts. Through the proposed methodology, it was demonstrated that the statistical approach suggested ensures consistent and robust ranking of alternatives; thereby identifying lactic acid as the best potential environmentally sustainable alternative within the design space.
A study of temperature sensor location based on fractal analysis for cascade control schemes in tubular reactors

Temperature sensor location for cascade control schemes in tubular reactors is still an open research problem. Several studies have pointed out that most temperature sensitive zones along the length of the reactor are suitable to this end. In this work, we have studied the problem of sensor location in a cascade control configuration using fractal analysis of time series obtained by random forcing of the jacket rector. A benchmark dispersion axial model displaying different temperature profiles is used to illustrate our findings.
A Systematic Approach to Explorative Scenario Analysis in Emergy Assessment with Emphasis on Resilience

Fossil energy depletion (specifically peak oil) and climate change are imagined to profoundly affect human civilisation. This motivates assessment of resilience, a concept associated with the ability to persist and maintain function. Explorative scenarios may be used to cast light on what the future may bring. We develop a systematic approach to explorative scenario analysis and attempt to quantify aspects of resilience specifically for emergy assessment (EmA) of production systems. We group system inputs into five categories: (1) fossil fuels, their derivatives, metals and minerals, (2) on-site renewable inputs, (3) slowly renewable inputs, (4) direct labour and (5) indirect labour. We consider the existing EmA indicators of biophysical efficiency (the unit emergy value, UEV), the degree of dependence on free, renewable, natural flows of energy (%R) and the degree of dependence on local inputs (%Local) as relevant resilience indicators in EmA. Formulas to calculate the corresponding indicators for the outputs in future scenarios are provided, e.g. the resulting adjustment factor for the UEV. We demonstrate our approach by parameterising four conceivable energy descent scenarios described by corresponding narratives. We analyse the aggregated effect on UEVs of these scenarios for production systems that differ with respect to how the emergy flow is distributed among the five input categories. We find that for most production systems, scenario conditions significantly affect the UEV. The production systems that rely primarily on on-site renewable resources appear less sensitive to societal changes. The significance of labour inputs varies among scenarios, and a higher percentage of labour inputs leads to increasing UEV in a Green Tech scenario but lower UEV in more radical energy descent scenarios. A comparison of two specific production systems showed that different expectations of the future lead to contrasting conclusions regarding prioritisation. We use the insight gained in the study to suggest venues for sustainable development under changing societal conditions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Kamp, A. (Intern), Østergård, H. (Intern)
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10.1016/j.ces.2015.10.036
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A Systematic Modelling Framework for Phase Transfer Catalyst Systems
Phase-transfer catalyst systems contain two liquid phases, with a catalyst (PTC) that transfers between the phases, driving product formation in one phase and being regenerated in the other phase. Typically the reaction involves neutral
species in an organic phase and regeneration involves ions in an aqueous phase. These reacting systems are receiving increased attention as novel organic synthesis options due to their flexible operation, higher product yields, and ability to avoid hazardous or expensive solvents. Major considerations in the design and analysis of PTC systems are physical and chemical equilibria, as well as kinetic mechanisms and rates. This paper presents a modelling framework for design and analysis of PTC systems that requires a minimum amount of experimental data to develop and employ the necessary thermodynamic and reaction models and embeds them into a reactor model for simulation. The application of the framework is made to two cases in order to highlight the performance and issues of activity coefficient models for predicting design and operation and the effects when different organic solvents are employed.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Korea Advanced Institute of Science & Technology, Universidad Autonoma Metropolitana, University of Virginia
Authors: Anantpinijwatna, A. (Intern), Sales-Cruz, M. (Ekstern), Hyung Kim, S. (Ekstern), O'Connell, J. P. (Ekstern), Gani, R. (Intern)
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BFI (2018): BFI-level 2
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.855 SNIP 1.449 CiteScore 2.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.957 SNIP 1.668 CiteScore 2.56
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.912 SNIP 1.335 CiteScore 2.12
ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 0.87 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.742 SNIP 1.029
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Atlantic salmon (Salmo salar) protein hydrolysate in diets for weaning piglets — effect on growth performance, intestinal morphometry and microbiota composition

Salmon protein hydrolysates (SPH) from two different raw materials were evaluated in diets for weaning piglets. Four experimental diets were included in the study: a diet based on plant protein with soy protein as the main protein source (Diet PP), a diet based on fishmeal in exchange for soy protein (Diet FM) and two diets in which different SPH replaced fishmeal in the FM diet. The experimental diets were fed to piglets from the day of weaning until 32 d postweaning. In addition to the record of performance data, an intestinal sampling for mucosal morphometry and microbiota 16S rRNA gene sequencing were performed at day 11 on a subset of the animals. The duodenal villi absorption area was significantly larger in piglets receiving Diets SPH compared with Diet PP (p < 0.02). A significant positive correlation between duodenal villi height and average daily gain during the first 11 d postweaning was detected. Only small differences in intestinal microbiota community and no differences in growth performance were detected between the experimental diets. To conclude, SPH seem to be an interesting novel protein source in weanling piglets.
MoO₃ has been tested as a catalyst in hydrodeoxygenation (HDO) of both model compounds (acetone and guaiacol) and real biomass pyrolysis vapors under atmospheric pressure. The pyrolysis vapor was obtained by fast pyrolysis of wood or lignin in a continuous fast pyrolysis reactor at a fixed temperature of 500 °C, and it subsequently passed through a downstream, close coupled, fixed bed reactor containing the MoO₃ catalyst. The influences of the catalyst temperature and the concentration of H₂ on the HDO of the pyrolysis vapors were investigated. The level of HDO of the biomass pyrolysis vapors was not significant at temperatures below 400 °C. At 450 °C catalyst temperature and 93 vol % H₂ concentration, the wood pyrolysis vapor was more active toward cracking forming gas species instead of performing the desired HDO forming hydrocarbons. The lignin pyrolysis vapor was more resistant to cracking and yielded 16.2 wt %daf organic liquid, while achieving 52% degree of deoxygenation at 450 °C catalyst temperature under 89 vol % H₂ concentration. The corresponding energy recovery in the liquid phase was 23.5%. The spent catalyst showed two deactivation routes, coke formation and reduction of MoO₃ to MoO₂, which is inactive in HDO. The catalyst experienced severe reduction at temperatures higher than 400 °C. The yields of coke relative to the fed biomass were in the range of 3–4 wt %daf for lignin and 5–6 wt %daf for wood. Compared to untreated bio-oil the upgraded lignin organic liquid showed improved compatibility with hydrocarbons and was miscible with a toluene/heptane mixture.
Atmospheric plasma assisted PLA/microfibrillated cellulose (MFC) multilayer biocomposite for sustainable barrier application

Fully bio-based and biodegradable materials, such as polylactic acid (PLA) and microfibrillated cellulose (MFC), are considered in order to produce a completely renewable packaging solution for oxygen barrier applications, even at medium-high relative humidity (R.H.). Thin layers of MFC were coated on different PLA substrates by activating film surface with an atmospheric plasma treatment, leading to the fabrication of robust and transparent multilayer composite films, which were then characterized by different experimental techniques. UV transmission measurements confirmed the transparency of multilayer films (60% of UV transmission rate), while SEM micrographs showed the presence of a continuous, dense and defect free layer of MFC on PLA surface. Concerning the mechanical behavior of the samples, tensile tests revealed that the multilayer films significantly improved the stress at break value of neat PLA. Moreover, the oxygen barrier properties of the multilayer films were improved more than one order of magnitude compared to neat PLA film at 35. °C and 0% R.H. and the permeability values were maintained up to 60% R.H. The obtained materials therefore showed interesting properties for their possible use in barrier packaging applications as fully biodegradable solution, coupling two primarily incompatible matrices in a multilayer film with no need of any solvent or chemical.
Automatic Functionality Assignment to AUTOSAR Multicore Distributed Architectures

The automotive electronic architectures have moved from federated architectures, where one function is implemented in one ECU (Electronic Control Unit), to distributed architectures, where several functions may share resources on an ECU. In addition, multicore ECUs are being adopted because of better performance, cost, size, fault-tolerance and power consumption. In this paper we present an approach for the automatic software functionality assignment to multicore distributed architectures. We consider that the systems use the AUTomotive Open System ARchitecture (AUTOSAR). The functionality is modeled as a set of software components composed of subtasks, called runnables, in AUTOSAR terminology. We have proposed a Simulated Annealing metaheuristic optimization that decides: (i) the mapping of software components to multicore ECUs, (ii) the assignment of runnables to the ECU cores, (iii) the clustering of runnables into tasks and (iv) the mapping of tasks to “OS-Applications” (used to isolate mixed safety-criticality functions). We are interested to determine an implementation such that (1) the mapping constraints are satisfied, (2) the runnables are schedulable and (3) they are spatially and temporally isolated if they have different safety-criticality levels, (4) the overall communication bandwidth is minimized and (5) the utilization of the cores and ECUs is balanced. The proposed approach was evaluated on three realistic case studies.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Copenhagen Center for Health Technology, Department of Applied Mathematics and Computer Science, Embedded Systems Engineering, Volvo Group Trucks Technology
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A viable electrode material for use in microbial fuel cells for tropical regions
Electrode materials are critical for microbial fuel cells (MFC) since they influence the construction and operational costs. This study introduces a simple and efficient electrode material in the form of palm kernel shell activated carbon (AC) obtained in tropical regions. The novel introduction of this material is also targeted at introducing an inexpensive and durable electrode material, which can be produced in rural communities to improve the viability of MFCs. The maximum voltage and power density obtained (under 1000 Ω load) using an H-shaped MFC with AC as both anode and cathode electrode material was 0.66 V and 1.74 W/m3, respectively. The power generated by AC was as high as 86% of the value obtained with the extensively used carbon paper. Scanning electron microscopy and Denaturing Gradient Gel Electrophoresis (DGGE) analysis of AC anode biofilms confirmed that electrogenic bacteria were present on the electrode surface for substrate oxidation and the formation of nanowires.

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Behavior of Alkali Metals and Ash in a Low-Temperature Circulating Fluidized Bed (LTCFB) Gasifier

A low-temperature circulating fluidized bed system (LTCFB) gasifier allows for pyrolysis and gasification to occur at low temperatures, thereby improving the retention of alkali and other inorganic elements within the system and minimizing the amount of ash species in the product gas. In addition, the low reactor temperature ensures that high-alkali biomass fuels can be used without risk of bed defluidization. This paper presents the first investigation of the fate of alkali metals and ash in low-temperature gasifiers. Measurements on bed material and product gas dust samples were made on a 100 kW and a 6 MW LTCFB gasifier. Of the total fuel ash entering the system, the largest fraction (40–50%) was retained in the secondary cyclone bottoms, while a lower amount (8–10%) was released as dust in the exit gas. Most of the alkali and alkaline earth metals were retained in the solid ash, along with Si and a minor fraction of Cl. Most Cl and S were released in gaseous form, with chlorine partly as methyl chloride. The tar in the product gas from the LTCFB gasifier contained only negligible amounts of potassium and other inorganic elements. The release of condensed ash species from the system was controlled by the particle size and the cut size of the primary and secondary cyclones. A model accounting for the ash collection by the plant cyclones was shown to predict the product gas ash particle release reasonably well.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Pyroneer A/S
Benchmarking of Processes for the Biosynthesis of Natural Products

Natural products constitute an extensive family of organic molecules with more than 200,000 compounds discovered in several natural sources (plants and microbes). Most of these compounds have a very complex structure, multiple chiral centers and can have different biological activities. These biological activities can be of interest for use in different sectors of chemical industry, in particular pharmaceutical industry where several drugs are derived or inspired by natural products structure.

However, the large scale production of natural products is hindered by its relatively poor abundance in nature, which makes extraction from natural sources an economically unfeasible technology in most of the cases. Chemical synthesis is also very difficult given the structural complexity and chirality of the molecules.

Synthetic biology offers very promising tools for production of natural products. Genetic engineering allows expressing the genes responsible for the biosynthesis of these natural products and to insert them into fermentable organisms like yeast or bacteria. And protein engineering offers the possibility to engineer the enzymes that perform the natural products' biosynthesis, which allows the production of these complex molecules in single or multi-steps biocatalytic reactions.

In this thesis, a systematic approach for route selection and screening of the different process options to manufacture a natural product is presented. This methodological approach includes a set of evaluation tools to assess processes both from an economic and environmental perspectives and it is demonstrated with two case-studies. For each case-study different tools are used to evaluate the process.

The first case-study consists of the bioconversion of (R)-limonene to (R)-perillic acid by *Pseudomonas putida* GS1. (R)-perillic acid is a monoterpenoic acid with antimicrobial properties. It has a strong inhibitory effect on bacteria and fungus, which makes it an attractive compound to be used as a preservative for instance in cosmetic industry, but on the other hand makes the biosynthesis a complicated process to develop. An environmental assessment of the different synthetic routes for (R)-perillic acid production showed that biosynthesis represents the most promising option. This process was further explored through an economic assessment and process modelling including a sensitivity analysis on key process metrics, which allowed the identification of the main process bottlenecks. Product inhibition and substrate loss were identified as some of the main process limitations and strategies for improving them were suggested.

The second case-study describes the production of a recombinant protein, brazzein, by fermentation of the yeast *Pichia pastoris*. Brazzein is a natural sweetener found in the fruits of the African plant *Pentadiplandra brazzzena* Baillon, which is sweeter than regular sucrose by several orders of magnitude. Here different tools were applied to evaluate the environmental profile of the process in comparison with other sweeteners.

The main benefit of this early-stage evaluation is putting the biosynthesis of natural products into context in relation to demands of an industrially feasible chemical process. Moreover, it can give very meaningful insight into process development and provides a good overview of the whole reaction and process. The proposed in silico approach can guide research and development and ultimately contribute to the implementation of more bioprocesses for the production of natural products.

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Organisations: PROSYS - Process and Systems Engineering Centre, Department of Chemical and Biochemical Engineering, KT Consortium
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Publication date: 2016

Bimodal condensation silicone elastomers as dielectric elastomers
Lately, dielectric elastomers (DEs) which consist of an elastomer sandwiched between electrodes on both sides, have gained interest as materials for actuators, generators, and sensors. An ideal elastomer for DE uses is characterized by high extensibility, flexibility and good mechanical fatigue as well as high electrical and mechanical breakdown strengths.

[1] Most model elastomers are prepared by an end-linking process using a crosslinker with a certain functionality $f$ and a linear polymer with functional groups in both ends, and the resulting networks are so-called unimodal networks where unimodal refers to that there is one polymer only in the system. As an alternative to unimodal networks there are the bimodal networks where two polymers with significantly different molecular weights are mixed with one crosslinker.
Silicone rubber can be divided into condensation type and addition type according to the curing reaction. The advantages of condensation silicones compared to addition are the relatively low cost, the curing rate largely being independent of temperature, the excellent adhesion, and the catalyst being nontoxic. In this work, a series of bimodal condensation silicone elastomers were prepared by mixing different mass ratios (9:1, 8:2, 7:3, 6:4, 5:5, 4:6) between long polydimethylsiloxane (PDMS) chains and short PDMS chains. The resulting elastomers were investigated with respect to their rheology, dielectric properties, tensile strength, electrical breakdown, as well as thermal stability. The bimodal elastomers reinforce themselves at large strain and the high electrical breakdown strength is obtained due both to the low extensibility of the short chains that attach strongly the long chains and to the extensibility of the last ones that retards the rupture process. Moreover, a series of elastomers with the same mass ratio (7:3) between long and short PDMS chains were made at different humidity (90%, 70%, 50%, 30%, 10%) at 23°C. The dielectric and mechanical properties of the resulting elastomers were shown to depend strongly on the atmospheric humidity level. In addition, the top and bottom surfaces of the elastomer (7:3) prepared at 23°C and 50% humidity were tested by water contact angle and optical microscope. The results show the bimodal condensation elastomer possesses structural heterogeneity, which may lead to favourable properties for DE applications.
Bioinspired Multifunctional Membrane for Aquatic Micropollutants Removal

Micropolllutants present in water have many detrimental effects on the ecosystem. Membrane technology plays an important role in the removal of micropolllutants, but there remain significant challenges such as concentration polarization, membrane fouling, and variable permeate quality. The work reported here uses a multifunctional membrane with rejection, adsorption, and catalysis functions to solve these problems. On the basis of mussel-inspired chemistry and biological membrane properties, a multifunctional membrane was prepared by applying "reverse filtration" of a laccase solution and subsequent "dopamine coating" on a nanofiltration (NF) membrane support, which was tested on bisphenol A (BPA) removal. Three NF membranes were chosen for the preparation of the multifunctional membranes on the basis of the membrane properties and enzyme immobilization efficiency. Compared with the pristine membrane, the multifunctional membrane exhibited significant improvement of BPA removal (78.21 ± 1.95%, 84.27 ± 7.30%, and 97.04 ± 0.33% for NT103, NF270, and NF90, respectively), all of which are clearly superior to the conventional Fenton treatment (55.0%) under similar conditions and comparable to soluble laccase coupled with NF270 membrane filtration (89.0%). The improvement would appear to be due to a combination of separation (reducing the enzymatic burden), adsorption (enriching the substrate concentration as well as prolonging the residence time), and lastly, catalysis (oxidizing the pollutants and breaking the "adsorption saturation limits"). Furthermore, the synergistic effect of the polydopamine (PDA) layer on the enzymatic oxidation of BPA was confirmed, which was due to its enhanced adsorption and electron transfer performance. The multifunctional membrane could be reused for at least seven cycles with an acceptable activity loss, demonstrating good potential for removal of micropolllutants.
Biomass-Ash-Induced Agglomeration in a Fluidized Bed. Part 1: Experimental Study on the Effects of a Gas Atmosphere

Fluidized beds have been widely applied to gasification and combustion of biomass. During gasification, a high temperature is preferable to increase the carbon conversion and to reduce the undesirable tar. However, the high temperature may lead to a severe agglomeration problem in a fluidized bed. Understanding of the agglomeration in various atmospheres is crucial to optimize the design and operation conditions. This study focuses on the effects of gases on agglomeration tendency with different types of biomass, including corn straw, rice straw, and wheat straw. The biomass ash samples are mixed with quartz sand and fluidized by the gas mixtures of N₂/CO₂, N₂/H₂, and N₂/steam or by air. At 550 °C, the bed temperature is increased at the rate of 3 °C/min until defluidization occurs. In this way, the defluidization temperature can be determined, which represents the agglomeration tendency. The agglomerates are analyzed by scanning electron microscopy–energy-dispersive X-ray spectrometry (SEM–EDS) for morphology and elemental composition. Significant differences are observed on the defluidization temperature (Tₐ) and agglomeration mechanisms in different gas atmospheres. Tₐ in H₂ and steam atmospheres are much lower than that in air. It appears that, in a steam atmosphere, the agglomeration of corn straw and rice straw ash is predominantly coating-induced. The agglomeration in both H₂ and air atmospheres are melting-induced. In a H₂ atmosphere, K₂SO₄ in the ash samples disappears, caused by decomposition of K₂SO₄.
Bioprocess Development of (R)-Perillic Acid Production with a Whole-Cell Biocatalyst

General information
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Bringing the life cycle perspective into the Cradle-to-Cradle certification: the case study of aluminium cans

General information
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Organisations: Department of Chemical and Biochemical Engineering, Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Niero, M. (Intern), Olsen, S. I. (Intern), Laurent, A. (Intern)
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Brittle fracture in associative polymers: the case of ionomer melts
Ionomers are interesting due to their applications in coatings, adhesives, films and packaging materials. A study of the underlying mechanisms for fracture in ionomers is consequently of both practical as well as theoretical interest. In this study, we employ high speed imaging coupled with uniaxial extensional rheometry to delineate the mechanics leading to the brittle fracture of ionomer melts. When these ionomers are elongated at a rate higher than the inverse relaxation time of physical crosslinks, an edge fracture occurs at a critical stress. Parabolic fracture profiles provide evidence that the phenomenon is purely elastic and bulk dissipation has little impact on the crack profile. Experimental results are interpreted within the Griffiths theory for linear elastic materials and the de Gennes theory for viscoelastic materials.

General information
State: Published
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Scopus rating (2012): SJR 1.898 SNIP 1.155 CiteScore 3.96
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Brown seaweed processing: enzymatic saccharification of Laminaria digitata requires no pre-treatment

This study assesses the effect of different milling pre-treatments on enzymatic glucose release from the brown seaweed Laminaria digitata having high glucan (laminarin) content. Wet refiner milling, using rotating disc distances of 0.1–2 mm, generated populations of differently sized pieces of lamina having decreasing average surface area (100–0.1 mm$^2$) with increased milling severity. Higher milling severity (lower rotating disc distance) also induced higher spontaneous carbohydrate solubilization from the material. Due to the seaweed material consisting of flat blades, the milling did not increase the overall surface area of the seaweed material, and size diminution of the laminas by milling did not improve the enzymatic glucose release. Milling was thus not required for enzymatic saccharification because all available glucose was released even from unmilled material. Treatment with a mixture of alginate lyase and a cellulase preparation (Cellic®CTec2) on large-sized milled material released all available glucose within 8 h. Application of the cellulase preparation alone released only half of the available glucose. The alginate lyase catalysis apparently induced selective removal of alginate to improve the cellulase catalyzed degradation of laminarin and cellulose in the material.

General information
State: Published
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Carbohydrate degradation mechanisms and compounds from pretreated biomass

The formation of inhibitors during pretreatment of lignocellulosic feedstocks is a persistent problem, and notably the compounds that retard enzymatic cellulose conversion represent an obstacle for achieving optimal enzymatic productivity and high glucose yields. Compounds with many chemical functionalities are formed during biomass pretreatment, which gives possibilities for various chemical reactions to take place and hence formation of many new potential inhibitor compounds. This somehow overlooked contemplation formed the basis for the main hypothesis investigated in this work:

Hypothesis 1) Liquors from biomass pretreatment contain an array of hitherto unidentified cellulase* inhibitors that are believed to be reaction products from carbohydrate degradation.

(*cellulases include endo-cellulases, cellobiohydrolases, LPMO, and beta-glucosidase enzyme activities)

Furthermore the two following two hypotheses were tested.

Hypothesis 2). Formation of these inhibitor compounds can be prevented by protection of reactive chemical functionalities as revealed from their mechanisms for formation.

Hypothesis 3) Process parameters influence the amount and type of reaction products (from hypothesis 1) that are formed and in turn change inhibition.

In order to point out potent cellulase inhibitors, a solvent extraction based fractionation method was developed to separate compounds in liquid from pilot plant hydrothermal pretreatment of wheat straw. Via 2-butanone extraction a group of potent cellulase inhibitors were identified with LC-MS/MS to be oligophenolic compounds. 26 of the compounds were new and by considering the reaction mechanisms and synthesis routes for their formation it was revealed that xylose was heavily involved in their formation. The new oligophenolic cellulase inhibitors were suggested to be formed during hydrothermal pretreatment by xylose self-condensation reactions involving aldol condensations, 1,4 additions to α,β unsaturated carbonyl compounds, 3-keto acid decarboxylations and oxidations. In addition xylose reactions with phenolic lignin components were suggested.

The identification of the central role of xylose in the reaction routes for oligophenolic inhibitor formation led to the solution to protect the reactive anomeric center in xylose. Protection of the anomeric center in in situ generated xylose with ethylene glycol monobutyl ether, during pretreatment of wheat straw, reduced the level of oligophenolic compounds with 73 % compared to the original pretreatment and 41 % compared to the control.

When pretreatment severity was increased the amount of xylooligosaccharides decreased whereas the amount of oligophenolic compounds increased. No new degradation compounds were formed although the profile of the oligophenolic inhibitors changed. New dipentoses with hydroxylated oxane bicyclic moieties and feruloylated tripentoses are suggested also to play a role in inhibition, because LC-MS/MS analysis revealed the presence of these components in the liquid from hydrothermal pretreated wheat straw after enzymatic treatment.

It was found that formation of the oligophenolic degradation compounds were common across biomass sources as sugar cane bagasse and oil palm empty fruit bunches. These findings were in line with that the oligophenolic compounds arise from reactions involving xylose from hemicellulose in the biomass. Even though oligophenolic degradation compounds were common across biomasses, variations were found in biomass structural elements that were released during pretreatment. Pentoseoligosaccharides from sugar cane bagasse had a more acetylated substitution pattern than wheat straw, and in oil palm empty fruit bunches 4-hydroxybenzoic acid was identified to be a variation from a lignin structural elements released during pretreatment.

In conclusion it was found that the reactions taking place during pretreatment of biomass are complex and involve both degradation compounds and biomass structural elements. The present work has shed some light over the reactions and from this new insight a new type of pretreatment with anomeric protection was proposed and tested. The results open up for implementation of new types of pretreatments that hinder monosaccharide degradation to inhibitor compounds in lignocellulosic biomass processing.

General information

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DONG Energy A/S
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Carbon footprint of rice production under biochar amendment - a case study in a Chinese rice cropping system

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Carbonic Anhydrase Enhanced Carbon Capture: Kinetic Measurements and Pilot Plant Trials

In this study the effect of carbonic anhydrase addition on the absorption of CO₂ was investigated in a wetted wall column apparatus. Four different solvents: MEA (a primary amine), AMP (a sterically hindered primary amine), MDEA (a tertiary amine) and K₂CO₃ a carbonate salt solution were tested in concentrations from 5 to 50 wt%. Necessary mass transfer parameters such as liquid side mass transfer coefficient and solvent and enzyme reaction rates were determined in a temperature range from 298 to 328 K and benchmarked to a 30 wt% MEA solution. The study reveals that the addition of the enzyme carbonic anhydrase (CA) dramatically increases the liquid side mass transfer coefficient for 30 wt% MDEA and 15 wt% K₂CO₃, 30 wt% AMP has a moderate increase whereas 30 wt% MEA was unchanged. The results confirm that bicarbonate forming solvent which do not produce carbamate benefit from CA. The results reveal the impact of temperature in relation to CA. A temperature increase resulted in lower liquid side mass transfer rate for 30 wt% MDEA and 15 wt% K₂CO₃ but in higher rate for 30 wt% AMP. The overall first order enzyme reaction rate (s⁻¹) was linearly dependent on enzyme concentration for 30 wt% MDEA and 15 wt% K₂CO₃ at 313 K. The derived enzymatic reaction rate constant kenz (m³ kg⁻¹ s⁻¹) for 15 wt% K₂CO₃ at 313 K was about 9 times higher than for 30 wt% MDEA and 10 times higher than for 30 wt% AMP. Temperature and concentration did not observably influence the enzymatic reaction rate constant in the concentration range of 5 to 15 wt% K₂CO₃. The higher solvent concentration only led to a slightly higher reaction rate. A solution with 20 wt% K₂CO₃ had almost 3 times higher enzyme reaction rate compared to 15 wt% at 298 K and increased with temperature to almost 5 times faster at 328 K. The enzymatic reaction rate for MDEA decreased with both temperature and solvent concentration from 15 to 30 wt%. An increase to 50 wt% resulted in a decrease in reaction rate due to less water present.

Pilot plant campaigns were carried out for different solvents and conditions and the results were successfully modelled using intrinsic data obtained from the wetted-wall column experiments.

Catalytic Hydrodeoxygenation of Biomass Pyrolysis Vapor Model Compounds over Molybdenum Sulfide Catalysts: Influence of Support, H₂S and Water

Conventional fast pyrolysis of biomass produces a high yield of bio-oil through well-established technologies. The produced bio-oil must be further processed in order to decrease the content of oxygen (from 15-30 wt% down to <1 wt%) and thereby enhance important fuel properties such as heating value, acidity and stability. Upgrading of condensed pyrolysis oil is challenged by severe polymerization and coking upon heating. Instead, it is proposed to perform pyrolysis in the presence of hydrogen and an HDO catalyst for immediate stabilization and upgrading of reactive pyrolysis products. Downstream deep HDO potentially ensures removal of oxygen down to <1 wt%. A schematic diagram for such a process is shown in Figure 1. A simplified bench scale setup is being constructed at DTU Chemical Engineering with a planned commissioning in Spring 2016. With a capacity of 100 g/h solid biomass, the aim is to provide a proof-of-concept for the continuous conversion of solid biomass to low oxygen, fuel-grade bio-oil. In this contribution, a combined experimental, characterization and theoretical study of catalytic hydrodeoxygenation of biomass pyrolysis vapor model compounds over molybdenum sulfide catalysts is presented. The influence of support, H₂S and water on activity, selectivity and deactivation is investigated.

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Authors: Arndal, T. M. H. (Intern), Høj, M. (Intern), Pintos, D. G. (Ekstern), Studt, F. (Ekstern), Grunwaldt, J. (Ekstern), Gabrielsen, J. (Ekstern), Jensen, A. D. (Intern)
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Conventional fast pyrolysis of biomass produces a high yield of bio-oil through well-established technologies [1]. The produced bio-oil must be further processed in order to decrease the content of oxygen (from 15-30 wt% down to <1 wt%) and thereby enhance important fuel properties such as heating value, acidity and stability [1,2]. Upgrading of condensed pyrolysis oil is challenged by severe polymerization and coking upon heating. Instead, it is proposed to perform pyrolysis in the presence of hydrogen and an HDO catalyst for immediate stabilization and upgrading of reactive pyrolysis products. Downstream deep HDO potentially ensures removal of oxygen down to <1 wt%. A schematic diagram for such a process is shown in Figure 1. A simplified bench scale setup is being constructed at DTU Chemical Engineering with a planned commissioning in Spring 2016. With a capacity of 100 g/h solid biomass, the aim is to provide a proof-of-concept for the continuous conversion of solid biomass to low oxygen, fuel-grade bio-oil.

This paper aims at developing a benchmark simulation model to evaluate control strategies for the urban catchment and sewer network. Various modules describing wastewater generation in the catchment, its subsequent transport and storage in the sewer system are presented. Global/local overflow based evaluation criteria describing the cumulative and acute effects are presented. Simulation results show that the proposed set of models is capable of generating daily, weekly and seasonal variations as well as describing the effect of rain events on wastewater characteristics. Two sets of case studies explaining possible applications of the proposed model for evaluation of: 1) Control strategies; and, 2) System modifications, are provided. The proposed framework is specifically designed to allow for easy development and comparison of multiple control possibilities and integration with existing/standard wastewater treatment models (Activated Sludge Models) to finally promote integrated assessment of urban wastewater systems.
Implementation of microbial fuel cells (MFCs) for electricity production requires effective current generation from waste products via robust cathode reduction. Three cathode types using dissolved oxygen cathodes (DOCs), ferricyanide cathodes (FeCs) and air cathodes (AiCs) were therefore assessed using bioethanol effluent, containing 20.5 g/L xylose, 1.8 g/L arabinose and 2.5 g/L propionic acid. In each set-up the anode and cathode had an electrode surface area of 88 cm², which was used for calculation of the current density. Electricity generation was evaluated by quantifying current responses to substrate loading rates and external resistance. At the lowest external resistance of 27 and highest substrate loading rate of 2 g chemical oxygen demand (COD) per L day, FeC-MFC generated highest average current density (1630 mA/m²) followed by AiC-MFC (802 mA/m²) and DOC-MFC (184 mA/m²). Electrochemical impedance spectroscopy (EIS) was used to determine the impedance of the cathodes. It was thereby confirmed that the FeC-MFC produced the highest current density with the lowest internal resistance for the cathode. However, in a setup using bioethanol effluent, the AiC-MFC was concluded to be the most sustainable option since it does not require ferricyanide. The data offer a new add-on option to the straw biorefinery by using bioethanol effluent for microbial electricity production.

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- Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Systems Biology
- Authors: Sun, G. (Intern), Thygesen, A. (Intern), Meyer, A. S. (Intern)
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Characterization of free radicals by electron spin resonance spectroscopy in biochars from pyrolysis at high heating rates and at high temperatures

The concentration and type of free radicals from the decay (termination stage) of pyrolysis at slow and fast heating rates and at high temperatures (above 1000°C) in biomass char have been studied. A room temperature electron spin resonance spectroscopy study was conducted on original wood, herbaceous biomass, holocelluloses, lignin and their chars, prepared at high temperatures in a wire mesh reactor, an entrained flow reactor, and a tubular reactor. The radical concentrations in the chars from the decay stage range up between 7·10^{16} and 1.5·10^{18} spins g\(^{-1}\). The results indicated that the biomass major constituents (cellulose, hemicellulose, lignin) had a minor effect on remaining radical concentrations compared to potassium and silica contents. The higher radical concentrations in the wheat straw chars from the decay stage of pyrolysis in the entrained flow reactor compared to the wood chars were related to the decreased mobility of potassium in the char matrix, leading to the less efficient catalytic effects of potassium on bond-breaking and radical re-attachments. The high Si levels in the rice husk caused an increase in the char radical concentration compared to the wheat straw because the free radicals were trapped in a char consisting of a molten amorphous silica at heating rates of 10^3\text{ to }10^4\text{ K s}^{-1}. The experimental electron spin resonance spectroscopy spectra were analyzed by fitting to simulated data in order to identify radical types, based on g-values and line widths. The results show that at high temperatures, mostly aliphatic radicals (g = 2.0026-2.0028) and PAH radicals (g = 2.0027\text{ to }2.0031) were formed.

General information

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Copenhagen
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Understanding fast pyrolysis of biomass-derived materials is an important step in optimization of combustion processes. Similar to coal combustion, the fuel burn out is known to be influenced by the yield and reactivity of chars, produced during pyrolysis. The rapid heating of small biomass particles and the short residence time at high temperatures minimize the char yield and increase char reactivity. The differences in chemical composition of organic and inorganic matter between wood and herbaceous biomass affect the operational flexibility of power plants, and increase the complexity of mathematical models that can predict yields, composition and rates of product (char, tar, light gases) formation from fast pyrolysis. The modeling of cross-linking and polymerization reactions in biomass pyrolysis includes the formation of free radicals and their disappearance. Knowledge about these radical reactions is important in order to achieve the high fuel
conversion at short residence times. However, little is known about the extent of free radical reactions in pulverized biomass at fast pyrolysis conditions. The concentration and type of free radicals from the decay (termination stage) of pyrolysis at slow and fast heating rates and at high temperatures (above 100°C) in biomass char have been studied. A room-temperature electron spin resonance spectroscopy study was conducted on original wood, herbaceous biomass, holocelluloses, lignin and their chars, prepared at high temperatures in a wire mesh reactor, an entrained-flow reactor, and a tubular reactor. The radical concentrations in the chars from the decay stage range up between 7x10^18 and 1.5x10^19 spins g^-1. The results indicated that any differences in the biomass major constituents (cellulose, hemicellulose, lignin) had a minor effect on remaining radical concentrations compared to potassium and silica contents. The higher radical concentrations in the wheat straw chars from the decay stage of pyrolysis in the entrained flow reactor compared to the wood chars were related to the decreased mobility of potassium in the char matrix, leading to the less efficient catalytic effects of potassium on the bond-breaking and radical re-attachments. The high Si levels in the rice husk caused an increase in the char radical concentration compared to the wheat straw because the free radicals were trapped in a char consisting of a molten amorphous silica at heating rates of 10^3°C s^-1. The experimental electron spin resonance spectroscopy spectra were analyzed by fitting to simulated data in order to identify radical types, based on g-values and line widths. The results show that at high temperatures, mostly aliphatic radicals (g = 2.0026-2.0028) and PAH radicals (g = 2.0007-2.0031) were formed. Free radicals structure from the termination stage was modelled by density functional theory (DFT).

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Lulea University of Technology, University of Copenhagen
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Characterization of water-forming NADH oxidases for co-factor regeneration
Traditional chemical methods for alcohol oxidation are often associated with issues such as high consumption of expensive oxidizing agents, generation of metal waste and the use of environmentally undesirable organic solvents. Developing green, selective catalysts is therefore important from an environmental and economic perspective [1]. Alcohol dehydrogenases (ADH) offer one such alternative. However, the reaction requires the oxidized nicotinamide co-factor (NAD^+) that must be recycled due to its high cost contribution. One regeneration method that offers certain advantages is the oxidation of NADH using water forming NADH oxidases (NOX-2). The implementation of the ADH/NOX system for alcohol oxidation, however, requires consideration of several different issues. Enzyme activity and stability at relevant pH and temperature conditions, but also the tolerance to the substrates and products present (alcohols and aldehydes) are important properties to characterize. Importantly, inactivation by gas-liquid interfaces has been reported for some enzymes, such as the NOX from Lactococcus lactis[2]. Thus, investigating the sensitivity to bubbling is also highly important from a process development perspective.

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Circular economy: To be or not to be in a closed product loop? A Life Cycle Assessment of aluminium cans with inclusion of alloying elements
Packaging, representing the second largest source of aluminium scrap at global level, deserves a key role in the transition towards the circular economy. Life Cycle Assessment (LCA) of aluminium products has been typically based on one life cycle considering pure aluminium flows and neglecting the presence of alloying elements and impurities. However, this simplification undermines the potentials of using LCA to quantify the environmental performances of products in multiple loops, as required in the circular economy. This study aims to investigate the effects of including the actual alloy
composition in the LCA of aluminium can production and recycling, in order to understand whether a can-to-can (i.e. closed product loop) recycling should be promoted or not. Mass balance of the main alloying elements (Mn, Si, Cu, Fe) was carried out at increasing levels of recycling rate, corresponding to a temporal interval of five years. Different aluminium packaging scrap sources were considered: mixed packaging aluminium scrap and used beverage can scrap. The outcomes of the mass balance were used to quantify the amount of Mn and primary Al that needs to be reintegrated in each scenario according to the recycling rate and this information was further used to perform an LCA of 30 loops of aluminium can production and recycling, based on the actual alloy composition. The LCA revealed that the closed product loop option (considering used beverage can scrap) has lower climate change impacts over the other recycling scenario using mixed Al packaging scrap. The main recommendation from an LCA methodological point of view is to include the idea of multiple co-functions in the functional unit definition. To further improve the environmental performances of the aluminium beverage can sector towards circular economy implementation the key actions are: to reduce the weight of the lid, to develop methods to separate the body and lid at the point of collection, and to investigate the potentials of a closed supply chain loop for aluminium cans in terms of combined environmental and economic value creation.

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Organisations: Department of Chemical and Biochemical Engineering, Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Niero, M. (Intern), Olsen, S. I. (Intern)
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.262 SNIP 1.811 CiteScore 2.91
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Scopus rating (2009): SJR 1.143 SNIP 1.647
Four experimental campaigns with gasification and co-gasification of sewage sludge in LT-CFB gasifiers are conducted to investigate of potential benefits and problematic issues related to sewage sludge management by LT-CFB gasification. Therefore, it was decided to progress with sewage sludge in a series of experimental campaigns to provide a detailed understanding of the process and the quality of LT-CFB ashes for use as fertilizers. The general benefits and drawbacks of low temperature gasification compared to anaerobic digestion and incineration are briefly discussed in this regard.

In the first part of this study, the Low Temperature Circulating Fluidized Bed (LT-CFB gasifier) is described. The LT-CFB gasifier is a technology originally developed for pre-processing of biomass fuels like cereal straw. In popular terms, the LT-CFB gasification process separates the inorganic and organic fractions of the straw. The majority of the inorganic material is extracted in one or several different ash fractions and the organic material is converted into a hot combustible gas product, which is subsequently combusted in an adjacent boiler. This substantially reduces the influence of the fuels inorganic composition on the combustion properties. When combining LT-CFB gasification with existing dust-fired coal boilers, fossil fuels can be directly substituted with renewable fuels while reusing existing energy infrastructure. Currently, two operational LT-CFB gasifiers exist: A pilot scale facility with a thermal capacity (TH) of 100 kW and a demonstration unit of 6 MWTH. Both units are involved in the present study. Many different fuels have previously been tested in LT-CFB gasifiers and previous results from these experiments are described and evaluated with focus on the energy efficiency of the process and the quality of LT-CFB ashes for use as fertilizers. The general benefits and drawbacks of low temperature gasification compared to anaerobic digestion and incineration are briefly discussed in this regard.

Development and implementation of a method to screen for new fuel candidates for LT-CFB gasification is conducted, and 22 new potential fuel candidates are characterized and compared to 4 previously proven LT-CFB fuels. The investigated fuel candidates are categorized by their apparent suitability as LT-CFB fuels and various positive characteristics as well as potentially problematic issues are discussed. The overall conclusion from the fuel screening is that in a Danish context it is highly relevant to consider low temperature gasification of especially sewage sludge and manure fibers while the international perspective includes especially sugarcane bagasse, various residues from olive oil production and rice husks. Only five fuel candidates are considered as potentially very problematic for single fuel LT-CFB gasification: Fat separated from wastewater treatment, palm kernel shell residues, two animal meat and bone meal samples and wood pruning from Italian vineyards. The problems mainly relate to the proximate composition, ash sintering, char deposit formation and corrosion of steel surfaces during thermal tests. The fuel screening also includes a screening of P fertilizer quality of ashes and chars produced from thermal treatment of the different fuels, and significant differences were identified between the P fertilizer quality of ashes and chars. The fuel screening also involves an investigation of how analytically determined characteristics of three fuel mixes differ from the expected linear sum of the involved fuels' individual characteristics. The results indicate profound possibilities for optimizing fuel and ash characteristics by fuel mixing with regard to ash deposit formation and sintering as well as ash and char P fertilizer quality.

Of the 5 best candidates identified in the fuel screening, sewage sludge is found to be one of the most interesting as it is a locally as well as globally available resource with a large potential for optimized management compared to several of the currently applied management options. Proper management of sewage sludge holds a substantial potential for recovery of highly concentrated phosphorus (P) with good plant availability in ashes and chars from the thermal conversion. It is therefore decided to progress with sewage sludge in a series of experimental campaigns to provide a detailed investigation of potential benefits and problematic issues related to sewage sludge management by LT-CFB gasification. Four experimental campaigns with gasification and co-gasification of sewage sludge in LT-CFB gasifiers are conducted.
and the results on process performance and the quality of the gas product are compared to results from other studies on thermal gasification of sludge. The overall conclusion is that many different gasifier designs have been proven successfully on sewage sludge fuels and LT-CFB gasification is very well suited for gasification of sewage sludge as well as co-gasification of sewage sludge and cereal straw. The LT-CFB gasifier is found to yield the highest hot gas efficiency, carbon conversion rate and total system electrical efficiency of the assessed systems.

Examination of the fertilizer quality of ash substrates from thermal conversion of sewage sludge is a central part of this study. Fertilizer quality is addressed by comparing the elemental composition, PAH content and P plant availability of LT-CFB ashes from different gasification and co-gasification campaigns to ash and char samples from incineration and pyrolysis of sewage sludge as well as to their respective untreated sludge samples and a mineral P reference. In addition to the conventional thermal platforms, a process for postoxidation of pyrolysis chars and gasification ashes has been developed and the oxidized substrates are also included in the investigation. From the investigation of ash fertilizer quality it is concluded that all of the investigated thermal platforms are applicable for production of P fertilizers by conversion of sewage sludge with the proper design and operational settings. Post-oxidation of pyrolysis chars and gasification ashes is found to have a remarkable effect on P fertilizer quality while co-gasification of sludge and straw in LT-CFB gasifiers in general seem to provide a better ash fertilizer than mono-sludge gasification. Assessment of the influence of the thermal process on the fertilizer quality of the ashes is studied with chemical sequential extraction and scanning electron microscopy to identify changes in P association induced by different thermal treatments. Changes in P fertilizer quality as function of incubation time and as function of changes in the particle size distribution of the ash substrate is also discussed.

In the last part of the study, the results from the previous chapters are combined in an assessment of the possibilities to produce controlled release fertilizers and context-specific designer fertilizers in systems encompassing thermal conversion of secondary resources. A discussion about burden shifting in such management systems is also introduced and results are analyzed from two life cycle assessment case studies comparing sewage sludge gasification in centralized LT-CFB gasifiers with the current practice of direct application of sludge on farm soil. The results indicate a substantial improvement of the LT-CFB scenario compared to the reference case with regard to a reduced impact on climate change and reduced toxicity of the P fertilizer.

Based on this work it is concluded that there is a profound potential for optimizing the management of sewage sludge – and most likely also many other secondary resources, by applying the proper thermal processes. With a good match between fuel characteristics, process design and end use of the produce dash and gas products, such a system can be setup to encompass full utilization of the energy potential in the resource and simultaneously produce high quality fertilizers. LT-CFB gasification is in many respects a very promising platform for this purpose combining flexibility in fuels and products and high energy efficiency. Co-gasification of sewage sludge and cereal straw is found to produce very high quality thermally purified P fertilizers, and the potential benefits of fuel mixing needs to be further examined.
the biopretreatments did not improve the methane potential of the WS, but improved the initial biogas production rate significantly. Conclusion: The combination of the L. buchneri ensiling and C. subvermispora WRF treatment provided a significant improvement in the pretreatment effect on WS. This combined biopretreatment produced particularly promising results for ethanol production.

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Comparative analysis of experimental methods for quantification of small amounts of oil in water

During core flooding experiments where water is injected into oil bearing core plugs, the produced fluids can be sampled in a fraction collector. When the core approaches residual oil saturation, the produced amount of oil is typically small (can be less than a few microliters) and the quantification of oil is then difficult. In this study, we compare four approaches to determine the volume of the collected oil fraction in core flooding effluents. The four methods are: Image analysis, UV/visible spectroscopy, liquid scintillation counting, and low-field nuclear magnetic resonance (NMR) spectrometry. The procedure followed to determine the oil fraction and a summary of advantages and disadvantages of each method are given. Our results show that all four methods are reproducible with high accuracy. The NMR method was capable of direct quantification of both oil and water fractions, without comparison to a pre-made standard curve. Image analysis, UV/visible spectroscopy, and liquid scintillation counting quantify only the oil fraction by comparing with a pre-made standard curve. The image analysis technique is reliable when more than 0.1 ml oil is present, whereas liquid scintillation counting performs well when less than 0.6 ml oil is present. Both UV/visible spectroscopy and NMR spectrometry produced high accuracy results in the entire studied range (0.006-1.1 ml). In terms of laboratory time, the liquid scintillation counting is the fastest and least user dependent, whereas the NMR spectrometry is the most time consuming. (C) 2016 Elsevier B.V. All rights reserved.
Comparative analysis of the effect of pretreating aspen wood with aqueous and aqueous-organic solutions of sulfuric and nitric acid on its reactivity during enzymatic hydrolysis

The effect of aspen wood pretreatment methods with the use of both aqueous solutions of sulfuric and nitric acids and aqueous-organic solutions (ethanol, butanol) of sulfuric acid (organosolv) on the limiting degree of conversion of this type of raw material into simple sugars during enzymatic hydrolysis are compared. The effects of temperature, acid concentration, composition of organic phase (for sulfuric acid), and pressure (for nitric acid) on the effectiveness of pretreatment were analyzed. It is shown that the use of organosolv with 0.5% sulfuric acid allows us to increase the reactivity of ground wood by 300–400%, compared to the initial raw material. Pretreatment with a 4.8% aqueous solution of nitric acid (125°C, 1.8 MPa, 10 min) is shown to be most effective, as it increases the reactivity of the ground aspen wood by more than 500%.

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Comparison of high temperature chars of wheat straw and rice husk with respect to chemistry, morphology and reactivity

Fast pyrolysis of wheat straw and rice husk was carried out in an entrained flow reactor at high temperatures (1000-1500°C). The collected char was analyzed using X-ray diffractometry, N2-adsorption, scanning electron microscopy, particle size analysis with CAMSIZER XT, 29Si and 13C solid-state nuclear magnetic resonance spectroscopy and thermogravimetric analysis to investigate the effect of inorganic matter on the char morphology and oxygen reactivity. The silicon compounds were dispersed throughout the turbostratic structure of rice husk char in an amorphous phase with a low melting temperature (∼730°C), which led to the formation of a glassy char shell, resulting in a preserved particlesize and shape of chars. The high alkali content in the wheat straw resulted in higher char reactivity, whereas the lower silicon content caused variations in the char shape from cylindrical to near-spherical char particles. The reactivities of pinewood and rice husk chars were similar with respect to oxidation, indicating less influence of silicon oxides on the char reactivity.

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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.188 SNIP 1.368
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.521 SNIP 1.615 CiteScore 4.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.888 SNIP 1.985 CiteScore 4.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.678 SNIP 1.823 CiteScore 4.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Comparison of phosphorus recovery from incineration and gasification sewage sludge ash

In incineration of sewage sludge is a common practice in many western countries. Gasification is an attractive option because of its high energy efficiency and flexibility in the usage of the produced gas. However, they both unavoidably produce sewage sludge ash (SSA), a material which is rich in phosphorus (P), but that it is commonly landfilled or used in construction materials. With current uncertainty in phosphate rock (PR) supply, P recovery from SSA has become interesting. In the present work, ashes from incineration and gasification of the same sewage sludge were compared in terms of P extractability using electrodiagnostic (ED) methods. The results show that comparable recovery rates of P were achieved with a single ED step for incineration SSA and a sequential combination of two ED steps for gasification SSA, which was due to a higher influence of Fe and/or Al in P solubility for the latter. A product with lower level of metallic impurities and comparable to wet process phosphoric acid (WPA) was eventually obtained from gasification SSA. Thus, gasification becomes an interesting alternative to incineration also in terms of P separation.

General information

State: Published
Organisations: Department of Civil Engineering, ARTEK, Section for Arctic Engineering and Sustainable Solutions, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Computer-Aided Sustainable Process Synthesis-Design and Analysis

Process synthesis involves the investigation of chemical reactions needed to produce the desired product, selection of the separation techniques needed for downstream processing, as well as taking decisions on sequencing the involved separation operations. For an effective, efficient and flexible design approach, what is needed is a systematic way to identify the types of tasks-operations that need to be performed, the corresponding design of the operation-equipment, their configuration, mass-energy flows, etc., giving an optimal flowsheet. Due to the fact that process synthesis problems are by nature combinatorial and open ended, a number of different solution approaches have been proposed. However the solution for any synthesis-design problem is dependent on the search space of alternatives and the process performance criteria which in most cases are influenced by economic factors. This work focuses on the development and application of a computer-aided framework for sustainable synthesis-design and analysis of process flowsheets by generating feasible alternatives covering the entire search space and includes analysis tools for sustainability, LCA and economics. The synthesis method is based on group contribution and a hybrid approach, where chemical process flowsheets are synthesized in the same way as atoms or groups of atoms are synthesized to form molecules in computer aided molecular design (CAMD) techniques. The building blocks in flowsheet synthesis problem are called as process-groups, which represent a single or set of unit operations that are selected by employing a thermodynamic insights based method. These building blocks are then combined using connectivity rules to generate all the feasible flowsheet alternatives. The main advantage of representing the flowsheet with process-groups is that, the performance of the entire process can be evaluated from the contributions of the individual process-groups towards the selected flowsheet property (for example, energy consumed). The developed flowsheet property models include energy consumption, carbon footprint, product recovery, product purity etc. In this way, the entire list of feasible chemical process flowsheets are quickly generated, screened and selected for further analysis. In the next stage, the design of the most promising process flowsheet candidates is performed through a reverse simulation approach, where the design parameters of the unit operations in the process flowsheet are calculated from selected process-groups definition. In the next stage the selected design is analyzed, for identifying process limitations or bottlenecks (hot-spots) using a comprehensive analysis method consisting of economic, life cycle and sustainability factors that are translated into design targets. In the final stage the identified hot-spots are targeted for overall process improvement and to generate innovative designs.

In this work the developed framework along with the associated methods and tools is tested through three case studies related to both chemical and biochemical industry in order to ascertain the applicability of the framework. In each of the cases numerous alternatives of novel and designs reported by others are quickly generated and evaluated. In all the case studies tested, the final design generated by the framework was novel and more sustainable.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre
Authors: Kumar Tula, A. (Intern), Gani, R. (Intern), Huusom, J. K. (Intern)
Number of pages: 187
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Publication information
Place of publication: Kgs. Lyngby
Publisher: Danmarks Tekniske Universitet (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Anjan_Kumar_Tula_12_2016.pdf

Relations
Projects:
Computer-Aided Sustainable Process Synthesis-Design and Analysis
Publication: Research › Ph.D. thesis – Annual report year: 2017

Concurrent elevation of CO2, O3 and temperature severely affects oil quality and quantity in rapeseed

Plant oil is an essential dietary and bio-energy resource. Despite this, the effects of climate change on plant oil quality remain to be elucidated. The present study is the first to show changes in oil quality and quantity of four rapeseed cultivars in climate scenarios with elevated [CO2], [O3] and temperature (T) combined and as single factors. The combination of environmental factors resembled IPCC's 'business as usual' emission scenario predicted for late this century.
the climate scenarios reduced the average amounts of the six fatty acids (FAs) analysed, though in some treatments single FAs remained unchanged or even increased. Most reduced was the FA essential for human nutrition, C18:3-ω3, which decreased by 39% and 45% in the combined scenarios with elevated [CO2]+T+[O3] and [CO2]+T, respectively. Average oil content decreased 3–17%. When [CO2] and T were elevated concurrently, the seed biomass was reduced by half, doubling the losses in FAs and oil content. This corresponded to a 58% reduction in the oil yield per hectare, and C18:3-ω3 decreased by 77%. Furthermore, the polyunsaturated FAs were significantly decreased. The results indicate undesirable consequences for production and health benefits of rapeseed oil with future climate change. The results also showed strong interactive effects of CO2, T and O3 on oil quality, demonstrating why prediction of climate effects requires experiments with combined factors and should not be based on extrapolation from single factor experiments.

General information
State: Published
Organisations: Department of Environmental Engineering, Department of Applied Mathematics and Computer Science, Statistics and Data Analysis, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Atmospheric Environment, Danish Cancer Society, University of Innsbruck
Pages: 4117-4125
Publication date: 2016
Main Research Area: Technical/natural sciences

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Journal: Journal of Experimental Botany
Volume: 67
Issue number: 14
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Web of Science (2013): Indexed yes
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Web of Science (2011): Indexed yes
ISI indexed (2011): ISI indexed yes
Web of Science (2010): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.336 SNIP 1.8
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.344 SNIP 1.698
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Scopus rating (2008): SJR 2.197 SNIP 1.528
Scopus rating (2007): SJR 2.274 SNIP 1.682
Conducting Polymeric Materials

The overall objective of this collection is to provide the most recent developments within the various areas of conducting polymeric materials. The conductivity of polymeric materials is caused by electrically charged particles, ions, protons and electrons. Materials in which electrons are the charge transfer elements are intrinsically conducting polymers, where the electrical conductivity is a result of delocalized electrons along the polymer backbone, with polyaniline, polypyrrole, and PEDOT as prominent examples. Already in 2000 Alan Heeger, Alan MacDiarmid, and Hideki Shirakawa were awarded the Nobel Prize in chemistry “for the discovery and development of conductive polymers”.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Hvilsted, S. (Intern)
Number of pages: 1
Pages: 1107
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Macromolecular Chemistry and Physics
Volume: 217
Issue number: 10
ISSN (Print): 1022-1352
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.58 SJR 0.949 SNIP 0.728
Web of Science (2016): Indexed yes
Consumer perceptions of the environmental sustainability of liquid food packaging: a survey among Danish consumers

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Management Engineering, Quantitative Sustainability Assessment, Technical University of Denmark
Authors: Niero, M. (Intern), Boesen, S. (Ekstern), Bey, N. (Intern)
Pages: 122
Publication date: 2016

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Main Research Area: Technical/natural sciences
Conference: 22nd SETAC Europe LCA Case Study Symposium , Montpellier, France, 20/09/2016 - 20/09/2016
Electronic versions:
LCA2016_programme_book_V4_DD.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016
Continuous anaerobic digestion of swine manure: ADM1-based modelling and effect of addition of swine manure fibers pretreated with aqueous ammonia soaking

Anaerobic digestion of manure fibers presents challenges due to their low biodegradability. Aqueous ammonia soaking (AAS) has been tested as a simple method to disrupt the lignocellulose and increase the methane yield of manure fibers. In the present study, mesophilic anaerobic digestion of AAS pretreated manure fibers was performed in CSTR-type digesters, fed with swine manure and/or a mixture of swine manure and AAS pretreated manure fibers (at a total solids based ratio of 0.52 manure per 0.48 fibers). Two different simulations were performed. In the first place, the Anaerobic Digestion Model 1 (ADM1) was fitted to a manure-fed, CSTR-type digester and validated by simulating the performance of a second reactor digesting manure. It was shown that disintegration and hydrolysis of the solid matter of manure was such a slow process that the organic particulate matter did not significantly contribute to the methane production. In the second place, ADM1 was used to describe biogas production from the codigestion of manure and AAS pretreated manure fibers. The model predictions regarding biogas production and methane content were in good agreement with the experimental data. It was shown that, AAS treatment significantly increased the disintegration and hydrolysis rate of the carbohydrate compounds of the fibers. The effect of the addition of AAS treated fibers on the kinetics of the conversion of other key compounds such as volatile fatty acids was negligible.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Aalborg University, Institute of Chemical Engineering Sciences, National Technical University of Athens
Authors: Jurado, E. (Ekstern), Antonopoulou, G. (Ekstern), Lyberatos, G. (Ekstern), Gavala, H. N. (Intern), Skiadas, I. V. (Intern)
Pages: 190-198
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Main Research Area: Technical/natural sciences

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Journal: Applied Energy
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.854 SNIP 3.108 CiteScore 5.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.473 SNIP 2.84 CiteScore 5.5
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.516 SNIP 2.25
Continuous production of chitooligosaccharides by an immobilized enzyme in a dual-reactor system

A chitosanolytic activity found in a commercial α-amylase from Bacillus amyloquefaciens (BAN) was covalently immobilized onto glyoxal agarose beads (25% recovery of activity) and assessed for the continuous production of chitooligosaccharides (COS). The immobilization did not change the reaction profile (with chitotriose and chitobiose as major products, using chitosans of different polymerization and deacetylation degrees), but significantly increased the enzyme thermostability. A two-step process was proposed, in which chitosan was first hydrolyzed in a batch reactor to a viscosity that could flow through a packed-bead reactor (PBR), thus avoiding clogging of the column. The relationship between hydrolysis degree of chitosan (1% w/v) and viscosity of the solution was assessed in a batch reactor. A 50% hydrolyzed chitosan did not cause any clogging of the PBR. Under these conditions, the productivity of the PBR at the lowest dilution rate was 37 gCOS L⁻¹h⁻¹ with a conversion yield of 73%. In contrast, at the highest dilution rate, the productivity was nearly 200 gCOS L⁻¹h⁻¹, but the conversion yield dropped to around 40%.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Instituto de Catálisis y Petroleoquímica
Authors: Santos-Moriano, P. (Ekstern), Woodley, J. (Intern), Plou, F. J. (Ekstern)
Pages: 211-217
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Molecular Catalysis B: Enzymatic
Volume: 133
ISSN (Print): 1381-1177
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
Controllability and flexibility analysis of CO2 post-combustion capture using piperazine and MEA

In this study, we developed a decentralized control scheme and investigate the performance of the piperazine (PZ) and monoethanolamine (MEA) CO2 capture process for industrially-relevant operation scenarios. The base for the design of the control schemes is Relative Gain Array (RGA) analysis combined with open-loop dynamic sensitivity analysis.

This study suggests that controllers with smaller time integrals and larger gains are required to maintain the PZ plant within reasonable short closed-loop settling times when compared to MEA. It also shows that the offset from the designated set-points in the presence of disturbances in the flue gas flow and heat duty is larger using PZ compared to MEA. The settling time for the PZ plant is generally larger than for MEA. However, the PZ plant rejects the disturbances...
faster and with less variability in the load of the power plant. Furthermore, this study indicates that the proposed PI-based control structure can handle large changes in the load provided that the manipulated variables, i.e. lean solvent flow or reboiler duty, do not reach their saturation limit. Additionally, we observed that shortage in the steam supply (reboiler duty) may represent a critical operational bottleneck, especially when PZ is being used. The MEA plant controllers drive the system towards drying out/flooding while the CO2 capture rate performance of the PZ plant reduces drastically in the presence of constraints in the availability of steam. These findings suggest the need for advanced control structures, e.g. MPC, which can explicitly account for constraints in the process variables.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, CERE – Center for Energy Resources Engineering, Copenhagen Center for Health Technology, Department of Chemical and Biochemical Engineering, University of Waterloo
Authors: Gaspar, J. (Intern), Ricardez-Sandoval, L. (Ekstern), Jørgensen, J. B. (Intern), Fosbøl, P. L. (Intern)
Pages: 276-289
Publication date: 2016
Main Research Area: Technical/natural sciences

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Volume: 51
ISSN (Print): 1750-5836
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.38 SJR 1.345 SNIP 1.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.515 SNIP 1.537 CiteScore 4.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.06 SNIP 2.412 CiteScore 4.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.331 SNIP 3.018 CiteScore 5.66
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.302 SNIP 1.987 CiteScore 4.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.499 SNIP 2.633 CiteScore 6.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.481 SNIP 2.436
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.058 SNIP 2.589
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.599 SNIP 1.172
Original language: English
Controllability, Flexible operation, Dynamic CO2 capture rate-based model, Piperazine, Sensitivity study
DOIs: 10.1016/j.ijggc.2016.06.003
Controlled retting of hemp fibres: Effect of hydrothermal pre-treatment and enzymatic retting on the mechanical properties of unidirectional hemp/epoxy composites

The objective of this work was to investigate the use of hydrothermal pre-treatment and enzymatic retting to remove non-cellulosic compounds and thus improve the mechanical properties of hemp fibre/epoxy composites. Hydrothermal pre-treatment at 100 kPa and 121 °C combined with enzymatic retting produced fibres with the highest ultimate tensile strength (UTS) of 780 MPa. Compared to untreated fibres, this combined treatment exhibited a positive effect on the mechanical properties of hemp fibre/epoxy composites, resulting in high quality composites with low porosity factor ($\alpha_{pf}$) of 0.08. Traditional field retting produced composites with the poorest mechanical properties and the highest $\alpha_{pf}$ of 0.16. Hydrothermal pretreatment at 100 kPa and subsequent enzymatic retting resulted in hemp fibre composites with the highest UTS of 325 MPa, and stiffness of 38 GPa with 50% fibre volume content which was 31% and 41% higher, respectively, compared to field retted fibres.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Wind Energy, Composites and Materials Mechanics, Technical University of Denmark, Swedish University of Agricultural Sciences
Authors: Liu, M. (Intern), Silva, D. A. S. (Ekstern), Fernando, D. (Ekstern), Meyer, A. S. (Intern), Madsen, B. (Intern), Daniel, G. (Ekstern), Thygesen, A. (Intern)
Pages: 253–262
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Composites Part A: Applied Science and Manufacturing
Volume: 88
ISSN (Print): 1359-835X
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.82 SJR 1.402 SNIP 2.053
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.53 SNIP 2.18 CiteScore 4.09
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.67 SNIP 2.538 CiteScore 4.08
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.59 SNIP 2.828 CiteScore 3.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.559 SNIP 2.706 CiteScore 3.36
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.443 SNIP 2.499 CiteScore 3.23
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.553 SNIP 2.241
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.536 SNIP 1.976
Control of wastewater N$_2$O emissions by balancing the microbial communities using a fuzzy-logic approach

In this work, a fuzzy-logic controller for minimization of the nitrous oxide emission from wastewater treatment plants is developed and tested in a simulation environment. The controller is designed in order to maintain a balance between production and consumption of nitrite by AOB and NOB microorganisms respectively. Thus, accumulation of nitrite is prevented and AOB denitrification, the main N$_2$O producer, is drastically slowed down. The controller is designed to adjust the oxygen supply according to a measured parameter which typically indicates the ratio of the activity of NOB over AOB. The controller is tested on a benchmark simulation model describing the production of N$_2$O during both AOB denitrification and HB denitrification. Comparisons between simulation results of open-loop and closed-loop have revealed the potential of the controller to significantly reduce the amount of N$_2$O emitted (approximately 35%). On the other side, this reduction of N$_2$O was accompanied by an increase in the aeration costs. Moreover, a plant performance evaluation under dynamic disturbances shows that the effluent quality is compromised due to higher requirements of organic carbon by denitrifying heterotrophs. The controller can therefore be considered effective for the reduction of N$_2$O production by AOB but would need to be coupled with a secondary control strategy ensuring a complete oxidation of the nitrogen oxides by heterotrophs to have a good effluent quality.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering
Authors: Boiocchi, R. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Pages: 1157-1162
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Main Research Area: Technical/natural sciences
Conference: 11th IFAC Symposium on Dynamics and Control of Process Systems Including Biosystems DYCOPS-CAB 2016 , Trondheim, Norway, 06/06/2016 - 06/08/2016
Fuzzy-logic, Benchmark, Nitrous oxide emission, Autotrophic denitrification, Nitrogen, wastewater treatment plants (WWTPs)
Electronic versions:
control_of_wastewater_N2O_emissions.pdf
DOIs:
10.1016/j.ifacol.2016.07.359
Source: FindIt
Source-ID: 2313798846
Control structure design for resource recovery using the enhanced biological phosphorus removal and recovery (EBP2R) activated sludge process

Nowadays, wastewater is considered as a set of resources to be recovered rather than a mixture of pollutants that should be removed. Many resource recovery schemes have been proposed, involving the use of novel technologies whose controllability is poorly studied. In this paper we present a control structure for the novel enhanced biological phosphorus removal and recovery (EBP2R) process, which is currently under development. The aim of the EBP2R is to maximize phosphorus recovery through optimal green micro-algal cultivation, which is achieved by controlling the nitrogen to phosphorus ratio (N-to-P ratio) fed to the algae. Process control structures are developed for a sequencing batch reactor (SBR) and a continuous flow reactor system (CFS). Results, obtained using the Benchmark Simulation Model No. 1 (BSM1) dynamic input disturbance time series, suggest that the SBR can maintain a stable N-to-P ratio in the effluent (16.9 ± 0.07) and can recover about 72% of the influent phosphorus. The phosphorus recovered by the CFS is limited by the influent nitrogen (65% of the influent phosphorus load). Using the CFS configuration the effluent N-to-P ratio cannot be effectively controlled (16.45 ± 2.48). Therefore, it is concluded that the SBR is the most effective reactor configuration for the EBP2R process. Importantly, the designed control structures rely on control loops that do not require chemical dosing for nutrient management, thereby reducing the environmental footprint of the EBP2R process. The proposed control strategies can be applied to other phosphorus recovery schemes where short sludge age EBPR systems play an important role.

General information
State: Published
Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
Authors: Valverde Perez, B. (Intern), Fuentes-Martínez, J. M. (Ekstern), Flores Alsina, X. (Intern), Gernaey, K. (Intern), Huusom, J. K. (Intern), Plósz, B. G. (Intern)
Pages: 447-457
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Journal
Volume: 296
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.34
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.92
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.96
ISI indexed (2011): ISI indexed yes
**CO₂ Capture Dynamic and Steady-State Model Development, Optimization and Control: Applied to Piperazine and Enzyme Promoted MEA/MDEA**

Despite the efforts and recent advances in renewable energy sources, the energy infrastructure is not yet ready to replace the fossil-fuel fired power plants with renewables. Thermal power plants represent the main energy supply and especially in developing countries, they are expected to dominate the market in the coming decades. However, the growing focus on mitigation of anthropogenic CO₂ requires integration of fossil-fuel fired power plant with CO₂ capture units. Post-combustion capture is the most mature capture technology and it is suitable for various processes in power plants, steel industry, cement production, and bio-chemical industry. However, to make CO₂ capture economically attractive, design of innovative solvents, optimization of operation conditions/process configuration and operational flexibility are of crucial importance.

This thesis aims to contribute to the development of efficient CO₂ post-combustion capture technology using alkanolamine solvents. Amine based CO₂ post-combustion capture is a reactive absorption process which implies complex mechanism of simultaneously occurring reaction and mass transport phenomena. Accordingly, first a simplified and easy to implement but general valid mass transfer model is developed and applied to single and parallel reactions systems, i.e. MEA, PZ and CA/MDEA. This mass transfer model uses existing correlations for mass and hydraulic characteristic and an enhancement factor to describe the acceleration of the mass transfer rate due to the reaction between CO₂ and amines. Afterwards, this sub-model together with the extended UNIQUAC thermodynamic model and correlations for physical properties is incorporated in a rate-based model for CO₂ absorption and desorption. The developed model is applied to MEA, PZ, PZ/K₂CO₃ and CA/MDEA and it is benchmarked against experimental pilot plant data and various models from independent research groups.

The validated steady-state model is used to determine set of optimal operation parameters for CO₂ capture post-combustion capture using PZ. This study accounts for the solubility window of PZ when determining the optimal and feasible operating conditions. The results are created in Aspen Plus using the hybrid CAPCO₂ rate-based user model. This model considers slurry formation in the calculation of CO₂ mass transfer rate. The results show how the capture process needs to be operated up to 14% above the minimum achievable heat duty, to avoid clogging from solid formation. 5 molal PZ is the most promising trade-off between energy efficiency and solid-free operation with a specific reboiler duty of 3.22 GJ/t CO₂ at 0.34 lean loading.

Furthermore, this thesis presents a dynamic rate-based model for CO₂ absorption and desorption using MEA and PZ as solvent. This dynamic model is an extension of the steady-state model as it uses the same thermodynamic-, mass transfer-, kinetic- and physical property- modules. These modules are implemented in Fortran and interfaced with the dynamic model which is implemented in Matlab. The developed model is used to investigate the transient behavior of a post-combustion plant using MEA and PZ. Moreover, a proportional-integral control structure is developed to investigate the controllability of the PZ based post-combustion plant compared to the MEA plant. The results reveal that PZ may be a better solvent than MEA as it can accommodate disturbances with less variability in the manipulated variables. However, control design alternatives and/or model based control structure should be developed to reduce the long settling time of the PZ plant compared to the MEA plant.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Energy production and transportation is responsible for more than 60% of our CO₂ emission. In particular, coal-fired power plants are big contributors. However, these large scale facilities offer the possibility to effective CO₂ capture through post-combustion processes. There are several options for such CO₂ capture. The problem is to make the absorption/desorption processes energetically and thereby economically viable. One process under investigation involves alkanoamines as absorbents in aqueous solutions. In these systems CO₂ is captured either by carbonate and/or carbamate formation. We have studied the 2-amino-2-methyl-1-propanol (AMP) and the AMP-water phase diagram and its ability for CO₂ capture. The first crystal structure in the AMP – water system has been solved from powder diffraction data: AMP trihydrate (triclinic, P-1, a = 6.5897(3), b = 6.399(2), c = 6.3399(2) Å and α = 92.40(3), β = 113.345(3) and γ = 94.06(2)°). In the AMP – water CO₂ system two structures, a carbamate, AMPH-AMPCO₂ and a carbonate, (AMPH)₂-CO₃ are known [1]. In this work we solved a new structure from powder diffraction data, AMPH-HCO₃ hydrate (monoclinic, I2/a, a = 21.8522(3), b = 6.2149(15), c = 12.1300(3) Å, β = 104.036(16)°) readily formed when using <40 at% AMP in water.

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Organisations: Department of Chemistry, X-ray Crystallography, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Ståhl, K. (Intern), Neerup, R. (Intern), Fosbøl, P. L. (Intern)
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Cyclic distillation technology - A mini-review
Process intensification in distillation systems has received much attention during the past decades, with the aim of increasing both energy and separation efficiency. Various techniques, such as internal heat-integrated distillation, membrane distillation, rotating packed bed, dividing-wall columns and reactive distillation were studied and reported in literature. All these techniques employ the conventional continuous counter-current contact of vapor and liquid phases. Cyclic distillation technology is based on an alternative operating mode using separate phase movement which leads to key practical advantages in both chemical and biochemical processes. This article provides a mini-review of cyclic distillation technology. The topics covered include the working principle, design and control methods, main benefits and limitations as well as current industrial applications. Cyclic distillation can be rather easily implemented in existing columns by simply changing the internals and the operating mode, thus bringing new life in old distillation towers by significantly increasing the column throughput, reducing the energy requirements and offering a better separation performance.
Data Handling and Parameter Estimation

Modelling is one of the key tools at the disposal of modern wastewater treatment professionals, researchers and engineers. It enables them to study and understand complex phenomena underlying the physical, chemical and biological performance of wastewater treatment plants at different temporal and spatial scales. At full-scale wastewater treatment plants (WWTPs), mechanistic modelling using the ASM framework and concept (e.g., Henze et al., 2000) has become an important part of the engineering toolbox for process engineers. It supports plant design, operation, optimization and control applications. Models have also been increasingly used to help take decisions on complex problems including the process/technology selection for retrofitting, as well as validation of control and optimization strategies (Gernaey et al., 2014; Mauricio-Iglesias et al., 2014; Vangsgaard et al., 2014; Bozkurt et al., 2015). Models have also been used as an integral part of the comprehensive analysis and interpretation of data obtained from a range of experimental methods from the laboratory, as well as pilot-scale studies to characterise and study wastewater treatment plants. In this regard, models help to properly explain various kinetic parameters for different microbial groups and their activities in WWTPs by using parameter estimation techniques. Indeed, estimating parameters is an integral part of model development and application (Seber and Wild, 1989; Ljung, 1999; Dochain and Vanrolleghem, 2001; Omlin and Reichert, 1999; Brun et al., 2002; Sinet et al., 2010) and can be broadly defined as follows: Given a model and a set of data/measurements from the experimental setup in question, estimate all or some of the parameters of the model using an appropriate statistical method.

The focus of this chapter is to provide a set of tools and the techniques necessary to estimate the kinetic and stoichiometric parameters for wastewater treatment processes using data obtained from experimental batch activity tests. These methods and tools are mainly intended for practical applications, i.e., by consultants, engineers, and professionals. However, it is also expected that they will be useful both for graduate teaching as well as a stepping stone for academic researchers who wish to expand their theoretical interest in the subject. For the models selected to interpret the experimental data, this chapter uses available models from literature that are mostly based on the Activated Sludge Model (ASM) framework and their appropriate extensions (Henze et al., 2000). The chapter presents an overview of the most commonly used methods in the estimation of parameters from experimental batch data, namely: (i) data handling and validation, (ii) parameter estimation: maximum likelihood estimation (MLE) and bootstrap methods, (iii) uncertainty analysis: linear error propagation and the Monte Carlo method.

Deactivation of Ni-MoS2 by bio-oil impurities during hydrodeoxygenation of phenol and octanol

The stability of Ni-MoS2/ZrO2 toward water, potassium, and chlorine containing compounds during hydrodeoxygenation (HDO) of a mixture of phenol and 1-octanol was investigated in a high pressure gas and liquid continuous flow fixed bed setup at 280 °C and 100 bar. To maintain the stability of the catalyst, sufficient co-feeding of a sulfur source was necessary to avoid oxidation of the sulfide phase by oxygen replacement of the edge sulfur atoms in the MoS2 structure. However, the addition of sulfur to the feed gas resulted in the formation of sulfur containing compounds, mainly thiols, in
the oil product if the residence time was too low. At a weight hourly space velocity (WHSV) of 4.9 h\(^{-1}\) the sulfur content in the liquid product was 980 ppm by weight, but this could be decreased to 5 ppm at a WHSV of 1.4 h\(^{-1}\). A high co-feed of sulfur was needed when water was present in the feed and the H\(_2\)O/H\(_2\)S molar ratio should be below ca. 10 to maintain a decent stability of the catalyst. Chlorine containing compounds caused a reversible deactivation of the catalyst when co-fed to the reactor, where the catalytic activity could be completely regained when removing it from the feed. Commonly, chlorine, H\(_2\)O, and H\(_2\)S all inhibited the activity of the catalyst by competing for the active sites, with chlorine being by far the strongest inhibitor and H\(_2\)S and H\(_2\)O of roughly the same strength. Dissimilar, potassium was a severe poison and irreversibly deactivated the catalyst to \(<5\%\) degree of deoxygenation when impregnated on the catalyst in a stoichiometric ratio relative to the active metal. This deactivation was a result of adsorption of potassium on the edge vacancy sites of the MoS\(_2\) slabs.

**General information**

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- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.303 SNIP 1.574 CiteScore 4.04
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- Web of Science (2013): Indexed yes
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- Scopus rating (2011): SJR 1.71 SNIP 1.706 CiteScore 4.15
- ISI indexed (2011): ISI indexed yes
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- Web of Science (2010): Indexed yes
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- Scopus rating (2009): SJR 1.761 SNIP 1.814
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
Defining carbohydrate binding of glucan phosphatases via Affinity gel electrophoresis

In plants, starch is the energy storage molecule that is readily broken down when needed. In animals, glycogen is the molecule that is used for energy storage. Both molecules are comprised of α-1, 4 linked glucose polymer chains and α-1,6 glucose branches that are tightly compacted. Our lab has determined the x-ray crystal structures of both plant and human glucan phosphatases and their enzymatic mechanisms. Despite this progress, we lacked the techniques to quickly and efficiently quantify their glucan phosphatase affinities for different substrates. The main objective of this study was to determine a technique to measure carbohydrate binding quickly and efficiently. We established a protocol to reproducibly and quantitatively measure the binding of the enzymes to glucans utilizing Affinity Gel Electrophoresis (AGE). The results show that the various glucan phosphatases possess differing abilities to bind to different glucan substrates. The plant glucan phosphatase SEX4 possesses a 50 fold higher affinity for the glucan amylopectin than LSF2, while SEX4 only possessed a 3 fold higher affinity for the glucan amylose than LSF2. Mutations were made to the various domains of the plant and animal glucan phosphatases to determine which regions of the enzyme are most necessary for binding.

Footnotes
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Defluidization in fluidized bed gasifiers using high-alkali content fuels

The major concern in thermal conversion of biomass encountered in fluidized beds is bed agglomeration, which may result in de-fluidization, leading to unscheduled downtime and additional costs. Biomass fuels, especially herbaceous plants, often contain significant amounts of silicon, potassium and calcium, which may form viscous melts that adhere on the surface of the colliding bed particles and bind them to form agglomerates. In this paper, studies were made to understand the behavior of inorganic elements (mainly K, Si and Ca) on agglomeration and de-fluidization of alkali rich bed-material samples under non-oxidizing conditions in a bench-scale fluidized bed reactor set up. The de-fluidization studies involved measurements with sand and pure potassium salts (KCl and K₂CO₃) as well as with bed material samples obtained from a 6 MW Low Temperature Circulating Fluidized Bed (LTCFB) gasifier using straw as a fuel. It was seen that in sand þ KCl agglomerates, the sand particles were bound by KCl melts. Only very limited chemical reaction was observed between KCl and the sand particles and no presence of silicate melts in the agglomerates. For sand þ K₂CO₃ mixtures and for LTCFB bed material samples, agglomeration could be attributed to viscous silicate melts formed from reaction of inorganic...
alkaline and alkali earth species with silica from the bed particles. A mathematical model that addresses the defluidization behavior of alkali-rich samples was developed based on the experiments performed in the bench-scale fluidized bed reactor as well as on results from literature. The model was then used to predict the de-fluidization behavior of alkali-rich bed material in a large-scale LTCFB gasifier.

**General information**

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**Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, DONG Energy A/S  
**Authors:** Narayan, V. (Intern), Jensen, P. A. (Intern), Henriksen, U. B. (Intern), Glarborg, P. (Intern), Lin, W. (Intern), Nielsen, R. G. (Ekstern)  
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  - BFI (2013): BFI-level 2  
  - Scopus rating (2013): SJR 1.678 SNIP 1.823 CiteScore 4.42  
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  - Scopus rating (2012): SJR 1.545 SNIP 1.743 CiteScore 3.66  
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  - Web of Science (2009): Indexed yes  
  - BFI (2008): BFI-level 2  
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  - Web of Science (2008): Indexed yes  
  - Scopus rating (2007): SJR 1.454 SNIP 1.77  
  - Web of Science (2007): Indexed yes  
  - Scopus rating (2006): SJR 1.292 SNIP 1.954  
  - Web of Science (2006): Indexed yes
Density and phase equilibrium of the binary system methane + n-decane under high temperatures and pressures

Densities of the binary system methane + n-decane have been determined through a vibrating tube densitometer from (278.15-463.15) K at pressures up to 140 MPa, and for methane mole fractions up to 0.8496. Negative excess volumes were found under the experimental conditions studied. Moreover isothermal compressibility values were obtained by differentiation from the Tammann-Tait correlation of the determined density values. Isobaric thermal expansion coefficients were also calculated based on differentiation from the isobaric fit of density data. We also measured the phase equilibrium of this binary system by using a variable volume cell with full visibility from (293.15-472.47) K for three mixtures with methane mole fractions of 0.4031, 0.6021 and 0.8496. Liquid fraction upon expansion below the saturation pressure has also been determined. Finally different equations of state were used to calculate the experimental density and excess volume data as well as the phase envelope data. No direct regression of the experimental data was involved in most of the calculation in order to provide a fair comparison of the performance of different models.
Deposit Shedding in Biomass-fired Boilers: Shear Adhesion Strength Measurements

Ash deposition on boiler surfaces is a major problem encountered during biomass combustion. Ash deposition adversely influences the boiler efficiency, may corrode heat transfer surfaces, and may even completely block flue gas channels in severe cases, causing expensive unscheduled boiler shutdowns. Therefore, timely removal of ash deposits is essential for optimal boiler operation. In order to improve the understanding of deposit shedding in boilers, this study investigates the shear adhesion strength of biomass ash deposits on superheater tubes. Artificial biomass ash deposits were prepared on superheater tubes and sintered in an oven at temperatures up to 1000 °C. Subsequently, the deposits were sheared off by an electrically controlled arm, and the corresponding adhesion strength was measured. The results reveal the effect of temperature, deposit composition, sintering duration, and steel type on the adhesion strength.

General information
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Determining optimum aging time using novel core flooding equipment

New methods for enhanced oil recovery are typically developed using core flooding techniques. Establishing reservoir conditions is essential before the experimental campaign commences. The realistic oil-rock wettability can be obtained through optimum aging of the core. Aging time is affected by temperature, crude oil, formation brine, and coreplug lithology. Minimum time can significantly reduce the experimental cost while insufficient aging time can result in false conclusions. Real-time online resistivity measurements of coreplugs are presented and a novel method is introduced for determining the optimum aging time regardless of variations in crude oil, rock, and brine properties. State of the art core flooding equipment has been developed that can be used for consistently determining the resistivity of the coreplug during aging and waterflooding using advanced data acquisition software. In the proposed equipment, independent axial and sleeve pressure can be applied to mimic stresses at reservoir conditions. 10 coreplugs (four sandstones and six chalk samples) from the North Sea have been aged for more than 408 days in total and more than 29000 resistivity data points have been measured to consistently investigate the change of wettability during aging. At 60°C and 100 bars a homogeneous sandstone coreplug attained optimized wettability after 5 days, a heterogeneous coreplug required 30 days of aging. Chalk coreplugs needed 45 days of aging. This shows that coreplugs originating from the same field, when aged at equivalent conditions can have significantly different aging times because of minor variations in the coreplug properties. No fixed aging time can be recommended on the other hand a method is recommended which can determine the extent of aging. Coreplug aging patterns were studied for variation in pressure (20 to 130 bar) and temperature (60 to 130°C).

Development of a Model for a Continuous Ultra-Filtration System

Due to the wide applicability and simplicity of the ultra-filtration process, it is currently being used in a variety of commercial processes for the purpose of separation and concentration of valuable products and/or recovery of raw materials from dilute systems [1]. A predictive model for a system derived from first principles, is instrumental in evading the costs of conducting time-consuming experiments while also allowing one to not be dependent on a trial and error analysis approach. The validated final model can serve to understand the operational issues of the process and from it identify the important phenomena occurring in the process and/or the corresponding model parameters. Also, it can help to
Twin-screw granulation is an emerging continuous granulation technique in the pharmaceutical industry. The flexibility in process settings such as the binder addition method (wet vs. dry), screw configuration, screw speed and material throughput allows to modify the granule size and shape. However, twin-screw granulation, being a rather new granulation technique, is not yet as well understood as batch-wise high shear wet granulation. Furthermore, most of the studies performed on twin-screw granulation are limited to a certain design and scale of the twin-screw granulator. In this study, in order to improve the understanding about the granulation process and to comprehend the applicability and limits of the process variables in a scale independent manner, the regime theory was applied to one specific twin-screw granulator equipment. In this study, α-lactose monohydrate was granulated with polyvinylpyrrolidone (2.5%, w/w) as binder. The connection equations were formulated to relate the retentate and permeate concentrations by the retentivity of the membrane.

Among the different models studied, the performance of a modified gel polarization model was identified and was found to yield good results. Experimental data from the literature was used to estimate the parameters of the model, i.e., the mass transfer coefficients and an operational parameter, the gelling concentration, could be estimated for each enzyme using a least-squares fit of the objective function. The mass transfer coefficient from theoretical relations is known to be a function of diffusion coefficient, velocity of flow and the membrane spacer dimensions. The diffusion coefficient, the most sensitive parameter of this model, was found to be a function of the feed concentration or the gelling concentration of the enzyme, depending on the operational scenario. This result also confirmed observations reported in published papers on this subject. Considering that, the velocity of flow and the membrane spacer dimensions are almost constant throughout the system, the mass transfer coefficient was found to vary only with the feed concentration. Lastly, the model was validated against experimental data and can predict the flow-rates within a difference of ±20% of the experimental data.

The presentation will provide details of the developed model; the modelling tool used to develop, analyse and solve the model equations; estimation and sensitivity analysis of important model parameters; and the comparison and validation of the model behaviour with published data.

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Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Novozymes A/S
Authors: Jhamb, S. V. (Intern), Gani, R. (Intern), Rype, J. (Ekstern), Wiklund, C. (Ekstern)
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Development of a process map: A step towards a regime map for steady-state high shear wet twin screw granulation
Twin-screw granulation is an emerging continuous granulation technique in the pharmaceutical industry. The flexibility in process settings such as the binder addition method (wet vs. dry), screw configuration, screw speed and material throughput allows to modify the granule size and shape. However, twin-screw granulation, being a rather new granulation technique, is not yet as well understood as batch-wise high shear wet granulation. Furthermore, most of the studies performed on twin-screw granulation are limited to a certain design and scale of the twin-screw granulator. In this study, in order to improve the understanding about the granulation process and to comprehend the applicability and limits of the process variables in a scale independent manner, the regime theory was applied to one specific twin-screw granulator equipment. In this study, α-lactose monohydrate was granulated with polyvinylpyrrolidone (2.5%, w/w) as binder. The screw configuration of the 25 mm diameter co-rotating twin-screw granulator from the ConsiGma-25 unit consisted of one or two kneading zones of six kneading elements each (1 x 6 and 2 x 6, respectively), at a stagger angle of 60. The specific mechanical energy, which involves the combination of screw speed, material throughput and torque required to rotate the screws, was correlated with the applied liquid-to-solid ratio to present process maps. The study suggested that, despite an increase in the granule size by the increasing liquid-to-solid ratio, most of the liquid contributes to formation of oversized granules. Therefore, keeping the liquid-to-solid ratio in a lower range and increasing the energy input to the system can be effectively used to lower the mean granule size. Changes in the screw geometry should also be explored to improve solid
liquid mixing and breakage of oversized granules to narrow the width of the size distribution. Since, such a process map is limited to a selected formulation and equipment design, process maps based on several formulations and mechanistic mathematical modelling tools should be applied to identify the mechanisms and relevant dimensionless groups that control granule attributes, with the ultimate aim of producing a generalised regime map. (C) 2015 Elsevier B.V. All rights reserved.

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Authors: Kumar, A. (Ekstern), Dhondt, J. (Ekstern), Vercruysse, J. (Ekstern), De Leersnyder, F. (Ekstern), Vanhoorne, V. (Ekstern), Vervaet, C. (Ekstern), Remon, J. P. (Ekstern), Gernaey, K. (Intern), De Beer, T. (Ekstern), Nopens, I. (Ekstern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.965 SNIP 1.598 CiteScore 2.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.89 SNIP 1.649 CiteScore 2.67
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.901 SNIP 1.875 CiteScore 2.64
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.854 SNIP 1.826 CiteScore 2.36
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.921 SNIP 1.86 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.94 SNIP 1.547
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.98 SNIP 1.65
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.911 SNIP 1.597
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.854 SNIP 1.316
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.118 SNIP 1.324
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.253 SNIP 1.399
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.867 SNIP 1.341
Scopus rating (2003): SJR 1.348 SNIP 1.489
Development of concepts for human labour accounting in Emergy Assessment and other Environmental Sustainability Assessment methods

Human labour is central to the functioning of any human-influenced process. Nevertheless, Environmental Sustainability Assessments (ESAs) do not systematically include human labour as an input. Systematic omission of labour inputs in ESAs may constitute an unfortunate, significant bias in favour of labour intensive processes and a systematic underestimation of environmental impacts has implications for decision-making. A brief review of the evaluation of human labour in ESAs reveals that only Emergy Assessment (EmA) accounts for labour as standard. Focussing on EmA, we find, however, that there is no agreement on the calculation method for labour. We formalise the calculation of human labour unit emergy values (UEVs) as being the ratio between the emergy resource basis of the labour system and a proxy for labour, with or without allocation to account for different qualities of labour. The formalised calculation approach is demonstrated using examples from the literature (USA, with allocation based on educational level; Ghana, with allocation based on income level; the World, with no allocation). We elaborate on how labour may be considered as endogenous or exogenous to the studied system, and how inputs can be categorised as direct labour taking place in the system under study and indirect labour occurring upstream in the supply chain associated with the studied system. With appropriate modifications, the formalised calculation approach and the distinction between direct and indirect labour may be transferred to other ESA methodologies. Concerning EmA, we recommend that product UEVs should systematically be calculated with and without labour, and that working hours rather than salary should be used when accounting for labour inputs. We recognise that there is a risk of double counting of environmental impacts when including labour. We conclude, however, that it can be ignored for most production systems, since only a negligible fraction of emergy already accounted for is likely to be included in the emergy flow from labour inputs.

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Authors: Kamp, A. (Intern), Morandi, F. (Intern), Østergård, H. (Intern)
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Scopus rating (2016): CiteScore 4.07 SJR 1.308 SNIP 1.756
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.481 SNIP 1.726 CiteScore 3.99
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.463 SNIP 1.996 CiteScore 3.76
BFI (2013): BFI-level 1
Devolatilization kinetics of woody biomass at short residence times and high heating rates and peak temperatures

This work combines experimental and computational fluid dynamics (CFD) results to derive global kinetics for biomass (pine wood) devolatilization during heating rates on the order of 10^5 Ks^-1, bulk flow peak temperatures between 1405 and 1667 K, and particle residence times below 0.1s. Experiments were conducted on a laboratory laminar entrained flow reactor (LFR) using solid fuel feed rates on the order of 10^-20 mgh^-1. Employing a simple single step first order (SFOR) mechanism with an Arrhenius type rate expression, the best fit of the pyrolysis kinetics was found to be: $A=18.9\times 10^3$ s^-1, $E_a=21305$ Jmol^-1. The accuracy of the derived global kinetics was supported by comparing predictions to experimental results from a 15kW furnace. The work emphasizes the importance of characterizing the temperature history of the biomass particles when deriving pyrolysis kinetics. The present results indicate faster kinetics than found in the literature, leading to predicted residence times required for full conversion one order of magnitude lower than when compared to thermogravimetric analysis (TGA) derived kinetics.

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Main Research Area: Technical/natural sciences

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Direct and inverse problems of infrared tomography

The problems of infrared tomography-direct (the modeling of measured functions) and inverse (the reconstruction of gaseous medium parameters)-are considered with a laboratory burner flame as an example of an application. The two measurement modes are used: active (ON) with an external IR source and passive (OFF) without one. Received light intensities on detectors are modeled in the direct problem or measured in the experiment whereas integral equations with respect to the absorption coefficient and Planck function (which yields the temperature profile of the medium) are solved in the inverse problem with (1) modeled and (2) measured received intensities as the input data. An axisymmetric flame and parallel scanning scheme of measurements considered in this work yield singular integral equations that are solved numerically using the generalized quadrature method, spline smoothing, and Tikhonov regularization. A software package in MATLAB has been developed. Two numerical examples-with modeled and real input data-were solved. The proposed methodology avoids the necessity of elaborate determination of the absorption coefficient by direct (point) measurements or calculation using spectroscopic databases (e.g., HITRAN/HITEMP). (C) 2015 Optical Society of America
Direct upgrading of fast pyrolysis lignin vapor over the HZSM-5 catalyst

Lignin has been pyrolyzed in a continuous fast pyrolysis reactor and the vapor was subsequently upgraded in situ over a downstream, close coupled HZSM-5 catalyst in a fixed bed reactor. The effect of the catalyst temperature on the HZSM-5 upgrading of lignin derived pyrolysis vapor was investigated. The results show that a high catalyst temperature (600 °C) is required in order to produce oxygen free aromatics. At a catalyst temperature of 600 °C, an organic liquid product, which contains 70 wt% oxygen free aromatics (mainly benzene and toluene), is obtained. However, the yield of the organic liquid is reduced from 27.6 wt%daf without a catalyst to 5.7 wt%daf (600 °C catalyst temperature). The energy recovery in the liquid organics is 8.7% (600 °C catalyst temperature), compared to the 33.0% energy recovery in the organic liquid from the non-catalytic run. Oxygen is removed from the pyrolysis vapor mainly in the form of H2O and CO when using the HZSM-5 zeolite, which is less optimal compared to if CO2 was the product. The organic liquid fraction, obtained from the 600 °C catalyst temperature experiment, has a low oxygen content of 4.0 wt%, compared to the 23.4 wt% oxygen content in the untreated organic liquid.
This work reveals new, important insights about the influence of broad spatial variation on the phylogenetic relationship and chemical characteristics of Ghanaian Hypnea musciformis—acarrageenan-containing red seaweed. DNA barcoding techniques alleviate the difficulty for accurate morphological identification. COI barcode sequences of the Ghanaian H. musciformis showed <0.7% intraspecies divergence, indicating no distinct phylogenetic variation, suggesting that they actually belong to the same species. Thus, the spatial distribution of the sampling sites along the coast of Ghana did not influence the phylogenetic characteristics of H. musciformis in the region. The data also showed that the Ghanaian Hypnea sp. examined in this work should be regarded as the same species as the H. musciformis collected in Brazilian Sao Paulo (KP725276) with only 0.8%–1.3% intraspecies divergence. However, the comparison of COI sequences of Ghanaian H. musciformis with the available COI sequence of H. musciformis from other countries showed intraspecies divergences of 0%–6.9% indicating that the COI sequences for H. musciformis in the GenBank may include different subspecies. Although samples did not differ phylogenetically, the chemical characteristics of the H. musciformis differed significantly between different sampling locations in Ghana. The levels of the monosaccharides, notably galactose (20%–30% dw) and glucose (10%–18% dw), as well as the seawater inorganic salt concentration (21–32 mg/L) and ash content (19%–33% dw), varied between H. musciformis collected at different coastal locations in Ghana. The current work demonstrated that DNA-based identification allowed a detailed understanding of H. musciformis phylogenetic characteristics and revealed that chemical compositional differences of H. musciformis occur along the Ghanaian coast which are not coupled with genetic variations among those samples.
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.624 SNIP 1.756
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.527 SNIP 1.604
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.38 SNIP 1.593
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.22 SNIP 1.524
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.308 SNIP 1.554
Scopus rating (2005): SJR 1.989 SNIP 1.262
Scopus rating (2004): SJR 1.464 SNIP 1.106
Scopus rating (2003): SJR 1.139 SNIP 1.188
Scopus rating (2002): SJR 0.944 SNIP 0.942
Scopus rating (2001): SJR 0.945 SNIP 1.256
Scopus rating (2000): SJR 0.672 SNIP 0.362
Scopus rating (1999): SJR 0.737 SNIP 1.002

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DNA barcodes, LSU, UPA, COI, Hypnea musciformis, Marine biodiversity, Carrageenan, Spatial variation, Seaweed, Phylogenetic, Ghana

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Bibliographical note
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Relations
Activities:
Seaweed Biorefinery in Ghana (SeaBioGha) (External organisation)
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Source-ID: 2305946355
Publication: Research - peer-review › Journal article – Annual report year: 2016

Downstream bioprocess characterisation within microfluidic devices
Miniaturising bioprocess unit operation steps is a well-established approach to find novel routes for process intensification and improved process economics. While a number of microbioreactors have been presented over the last 15 years, miniaturised downstream unit operations (mDUO) are less developed which has, to some extent, hindered their implementation as early process development tools. Microfluidic devices are particularly attractive for using fewer resources, for having the possibility of parallelisation and for requiring fewer mechanical manipulations. The expectation is that these devices will facilitate the rapid definition of critical process parameters, and thus ultimately reduce production costs.

We have developed several microfluidic mDUOs and combined them with advanced and novel analytical approaches, resulting in devices that can potentially be employed for both analytical and preparative purposes; these include devices for cross-flow filtration, liquid–liquid extraction and flocculation. To accelerate in-depth process characterisation, we developed and implemented on-line monitoring approaches and image-processing algorithms.

In this contribution, we will present results for the liquid–liquid extraction of pharmaceuticals, for the purification and concentration of drug delivery vehicles, and for the flocculation of yeast cells in microfluidic devices. For the latter, we will present for the first time the capability to study flocculation-growth independent from the floc breakage phase; two phases which are in a state of equilibrium in larger scale systems, and can thus not be discerned in conventional systems. The applicability of these devices will be shown with the assembly of a train of mDUO for the enzymatic production of chiral pharmaceutical intermediates.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University College London
Authors: Marques, M. (Ekstern), Krühne, U. (Intern), Szita, N. (Ekstern)
Number of pages: 1
Pages: S28
Dynamic Modeling and Analysis of an Industrial Gas Suspension Absorber for Flue Gas Desulfurization
In this work, semidry desulfurization of flue gas using a gas suspension absorber (GSA) is studied. A simple dynamic model which can properly represent the GSA was developed. In order to model the reaction kinetics, an empirical reaction rate expression was introduced. The reaction rate expression parameters were fitted to operational data from a real cement plant. A detailed statistical analysis of the parameter estimation procedure was performed, and the confidence intervals for estimated kinetic parameters were calculated. The model and reaction rate expression prediction ability was tested using another plant data set. It was verified that in spite of the simplicity of the model, very good prediction of industrial behavior was obtained. Furthermore, the dynamic analysis of the system was performed by carrying out open-loop and closed-loop simulations to verify plant dynamics. Therefore, a simple dynamic model with a reaction rate expression that is simple and efficient to use to predict the dynamics of GSA process was proposed in this work.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana, F.L. Smith A/S
Authors: Cignitti, S. (Intern), Mansouri, S. S. (Intern), Sales-Cruz, M. (Ekstern), Jensen, F. (Ekstern), Huusom, J. K. (Intern)
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Gas suspension absorber, Desulfurization kinetics, Dynamic modeling, Simulation, Control
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Dynamic modelling of nitrous oxide emissions from three Swedish sludge liquor treatment systems
The objective of this paper is to model the dynamics and validate the results of nitrous oxide (N₂O) emissions from three Swedish nitrifying/denitrifying, nitritation and anammox systems treating real anaerobic digestor sludge liquor. The Activated Sludge Model No. 1 is extended to describe N₂O production by both heterotrophic and autotrophic denitrification. In addition, mass transfer equations are implemented to characterize the dynamics of N₂O in the water and the gas phases. The biochemical model is simulated and validated for two hydraulic patterns: (1) a sequencing batch reactor; and, (2) a moving-bed biofilm reactor. Results show that the calibrated model is partly capable of reproducing the behaviour of N₂O as well as the nitritation/nitrification/denitrification dynamics. However, the results emphasize that additional work is required before N₂O emissions from sludge liquor treatment plants can be generally predicted with high certainty by simulations. Continued efforts should focus on determining the switching conditions for different N₂O formation pathways and, if full-scale data is used, more detailed modelling of the measurement devices might improve the conclusions that can be drawn.

General information
State: Published
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Dynamic Operation and Simulation of Post-Combustion CO₂ Capture

Thermal power need to operate, on a daily basis, with frequent and fast load changes to balance the large variations of intermittent energy sources, such as wind and solar energy. To make the integration of carbon capture to power plants economically and technically feasible, the carbon capture process has to be able to follow these fast and large load changes without decreasing the overall performance of the carbon capture plant. Therefore, dynamic models for simulation, optimization and control system design are essential. In this work, we compare the transient behavior of the model against dynamic pilot data for CO₂ absorption and desorption for step-changes in the flue gas flow rate. In addition we investigate the dynamic behavior of a full-scale post-combustion capture plant using monoethanolamine (MEA) and piperazine (PZ). This analysis demonstrates the good agreement between the developed model (dCAPCO₂) and the pilot measurements at both, transient and steady-state conditions. It outlines how the time needed to reach a new steady-state varies with respect to amine type and concentration. The simulation study reveals that it is essential to control the lean solvent flow to avoid sudden changes in the CO₂ removal rate and to avoid increased heat demand of solvent regeneration. In addition, it shows how storage tanks (liquid hold-up of the system) can be designed to accommodate significant upstream changes in the power plant management. This flexibility is especially needed for operation in future mixed green energy market. [All rights reserved Elsevier].

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Copenhagen Center for Health Technology, Department of Applied Mathematics and Computer Science, Scientific Computing, Technical University of Denmark
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BFI (2016): BFI-level 1
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.365 SNIP 0.561 CiteScore 0.92
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.425 SNIP 0.785 CiteScore 1.02
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.433 SNIP 0.957
Web of Science (2009): Indexed yes
Original language: English
Dynamic modeling, Flexible operation, Post-combustion CO₂ capture, Model validation, Pilot plant operations
Electronic versions:
Dynamic simulation and analysis of a pilot-scale CO2 post-combustion capture unit using piperazine and MEA

Post-combustion capture is a promising technology for developing CO2-neutral power plants. However, to make it economically and technically feasible, capture plants must follow the fast and large load changes of the power plants without decreasing the overall performance of the plant. Dynamic modeling and simulation is therefore needed to evaluate the performance of this plant under critical operation.

In this work, we evaluate the transient response of an absorber and a desorber for step changes of key process parameters, e.g. flue gas flow and composition, lean and rich CO2 loading, etc. We show the results for the baseline 30 wt% MEA and the low energy piperazine (PZ) solutions. This analysis reveals that the absorber reaches steady-state faster using MEA compared to PZ. This is related to the shift of the mass transfer zone due to changes in temperature. The transient operation in the regeneration unit is somewhat similar while using both solvents: an initial fast decrease of the lean loading is followed by a slow transient period as the system approaches steady-state conditions. We show the presence of inverse response in the stripper column when the rich loading decreases or the feed's temperature reduces using PZ solvent. Thus, we demonstrate that the dynamics of the MEA system cannot be extrapolated to other solvents.

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General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science , Scientific Computing, University of Waterloo
Authors: Gaspar, J. (Intern), Ricardez-Sandoval, L. (Ekstern), Jørgensen, J. B. (Intern), Fosbøl, P. L. (Intern)
Pages: 645-650
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Conference: 11th IFAC Symposium on Dynamics and Control of Process Systems Including Biosystems DYCOPS-CAB 2016, Trondheim, Norway, 06/06/2016 - 06/06/2016
Modelling and System Identification, Process Optimization and Plant wide Control, CO2 post-combustion capture
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Dynamics of Star Polymers in Fast Extensional Flow and Stress Relaxation

We confirm the observation from Ianniruberto and Marrucci [Macromolecules 2013, 46, 267-275] that entangled melts of branched polystyrenes behave like linear polystyrenes in the steady state of fast extensional flow, by measuring a linear, an asymmetric star, and a symmetric star polystyrene with the same span molecular weight (180 kg/mol). We show that all three melts reach the same extensional steady-state viscosity in fast extensional flow (faster than the inverse Rouse time).

We further measure stress relaxation following steady extensional flow for the three melts. We show that initially they relax in a similar way, most likely via arm retraction, at short time, but behave differently at long time due to both the length of the arm and the branch point. The terminal relaxation is described by a Doi and Edwards based model, i.e., considering pure orientational relaxation.

General information
Early-Stage Design and Analysis of Biorefinery Networks
The limited resources of fossil fuel as well as other important driving forces (e.g., environmental, social, and sustainability concerns) are expected to shape the future development of the chemical processing industries. These challenges motivate the development of new and sustainable technologies for the production of fuel, chemicals, and materials from renewable feedstock instead of fossil fuel. An emerging technology in response to these challenges is the biorefinery concept. The biorefinery is defined as the set of processes converting a bio-based feedstock into products such as fuels, chemicals, materials, and/or heat and power.

Economic risk analysis and critical comparison of optimal biorefinery concepts
In this paper, eight optimal biorefinery concepts for biofuels and biochemicals production are critically analyzed and compared in terms of their techno-economic performance and associated economic risks against historical market fluctuations. The investigated biorefinery concepts consider different combinations of biomass feedstock (lignocellulosic versus algal) and conversion technologies (biochemical versus thermochemical). In addition, the economic performance of each biorefinery concept is tested assuming a sudden drop in oil prices in order to compare the fitness/survival of each concept under extreme market disturbances. The analyses reveal amongst others that: (i) lignocellulosic bioethanol production is not economically feasible considering a drop in oil prices (a negative internal rate of return); (ii) a multi-product biorefinery concept, where bioethanol is upgraded to higher value-added chemicals (diethyl ether and 1,3-butadiene), provides an improved resilience and robustness against market price fluctuations by reducing economic loss by 140 MM$/a (17% IRR); (iii) the economic analysis favors biochemical conversion technologies for a small production/processing capacity, whereas the thermochemical conversion platform is favored for a relatively larger production capacity; and (iv) the microalgae-based biorefinery concept performed worse in terms of economics compared
to the others, which is largely due to the cost of algae production and harvesting. In general, we recommend that a comprehensive economic risk analysis, using for example the Monte-Carlo technique, should be an integral part of the conceptual design, development, and optimization of biorefineries to help improve their economic robustness in view of the competitive market for chemicals and fuels.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Utrecht University
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Scopus rating (2016): CiteScore 2.58 SJR 1.114 SNIP 1.291
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.643 SNIP 1.451 CiteScore 3.44
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.74 SNIP 1.704 CiteScore 3.92
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Scopus rating (2013): SJR 1.821 SNIP 1.867 CiteScore 4.49
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.487 SNIP 1.656 CiteScore 3.56
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.122 SNIP 2.284 CiteScore 4.68
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.046 SNIP 2.399
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.674 SNIP 2.237
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.97 SNIP 0.866

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Biorefinery, Process synthesis, Superstructure optimization, Economic analysis, Risk analysis

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10.1002/bbb.1654

**Economic Risk Assessment of Early Stage Designs for Glycerol Valorization in Biorefinery Concepts**

A systematic methodology to critically assess and screen among early stage design alternatives was developed for the use of glycerol. Through deterministic sensitivity analysis it was found that variations in the product and feedstock prices, total production cost, fixed capital investment, and discount rate, among others, have high impact on the project's profitability analysis. Therefore, the profitability was tested under uncertainties by using NPV and MSP as economic metrics. The robust ranking of solutions is presented with respect to minimum economic risk of the project being...
nonprofitable (failure to achieve a positive NPV times the consequential profit loss). It was found that the best potential options for glycerol valorization is through the production of either (i) lactic acid (9 MM$ with 63% probability of failure to achieve a positive NPV); (ii) succinic acid (14 MM$ with 76%); or finally, (iii) 1,2-propanediol (16 MM$ with 68%). As a risk reduction strategy, a multiproduct biorefinery is suggested which is capable of switching between the production of lactic acid and succinic acid. This solution comes with increased capital investment; however, it leads to more robust NPV and decreased economic risk by approximately 20%, therefore creating a production plant that can continuously adapt to market forces and thus optimize profitability.
Economic risk-based analysis: Effect of technical and market price uncertainties on the production of glycerol-based isobutanol

In this study, the production of glycerol-based isobutanol is critically assessed in terms of its techno-economic performance through the estimation of economic indicators, net present value (NPV) and minimum selling price (MSP). The Monte Carlo method with Latin Hypercube Sampling (LHS) is used to propagate the market price and technical uncertainties to the economic indicator calculations and to quantify the respective economic risk. The results clearly indicated that under the given market price uncertainties, the probability of obtaining a negative NPV is 0.95. This is a very high probability of failure, which corresponds to an economic risk of 20 MM$ as a potential loss. In order to decrease the economic risk, the integrated production of isobutanol as a module added to the biodiesel plant was tested as an alternative scenario. The probability of a negative NPV is decreased from 0.95 to 0.2 and the corresponding economic risk was reduced from 20 to 0.64 MM$. Using the integrated concept of utilising the waste glycerol stream in biodiesel plants contributes to the diversification of the product portfolio for vegetable oil based biorefineries, and in turn improves cost-competitiveness and robustness against market price fluctuations.
Effect of fast pyrolysis conditions on biomass solid residues at high temperatures

Fast pyrolysis of wood and straw was conducted in a drop tube furnace (DTF) and compared with corresponding data from a wire mesh reactor (WMR) to study the influence of temperature (1000-1400)°C, biomass origin (pinewood, beechwood, wheat straw, alfalfa straw), and heating rate (103 °C/s, 104 °C/s) on the char yield and morphology. Scanning electron microscopy (SEM), elemental analysis, and ash compositional analysis were applied to characterize the effect of operational conditions on the solid residues (char, soot) and gaseous products. The char yield from fast pyrolysis in the DTF setup was 3 to 7% (daf) points lower than in the WMR. During fast pyrolysis pinewood underwent drastic morphological transformations, whereas beechwood and straw samples retained the original porous structure of the parental fuel with slight melting on the surface. The particle size of Danish wheat straw char decreased in its half-width with respect to the parental fuel, whereas the alfalfa straw char particle size remained unaltered at higher temperatures. Soot particles in a range from 60 to 300 nm were obtained during fast pyrolysis. The soot yield from herbaceous fuels was lower than from wood samples, possibly due to differences in the content of lignin and resin acids.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Lulea University of Technology
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 4.15 SJR 1.416 SNIP 1.722
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.519 SNIP 1.822 CiteScore 4.09
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.629 SNIP 2.161 CiteScore 3.96
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.636 SNIP 2.142 CiteScore 3.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.682 SNIP 2.075 CiteScore 3.77
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.575 SNIP 1.773 CiteScore 3.38
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.629 SNIP 1.88
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Effect of pectin and hemicellulose removal from hemp fibres on the mechanical properties of unidirectional hemp fiber/epoxy composites

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Swedish University of Agricultural Sciences
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Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract M-17
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Effect of pectin and hemicellulose removal from hemp fibres on the mechanical properties of unidirectional hemp/epoxy composites

The objective of this study was to investigate the effect of pectin and hemicellulose removal from hemp fibres on the mechanical properties of hemp fibre/epoxy composites. Pectin removal by EDTA and endo-polygalacturonase (EPG) removed epidermal and parenchyma cells from hemp fibres and improved fibre separation. Hemicellulose removal by NaOH further improved fibre surface cleanliness. Removal of epidermal and parenchyma cells combined with improved fibre separation decreased composite porosity factor. As a result, pectin removal increased composite stiffness and ultimate tensile strength (UTS). Hemicellulose removal increased composite stiffness, but decreased composite UTS due to removal of xyloglucans. In comparison of all fibre treatments, composites with 0.5% EDTA + 0.2% EPG treated fibres had the highest tensile strength of 327 MPa at fibre volume content of 50%. Composites with 0.5% EDTA + 0.2% EPG → 10% NaOH treated fibres had the highest stiffness of 43 GPa and the lowest porosity factor of 0.04.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Swedish University of Agricultural Sciences
Effect of Platinum Group Metal Doping in Magnesium Diboride Wires

The effect of some platinum group metals (PGM = Rh, Pd, and Pt) on the microstructure and critical current density of Cu/Nb-sheathed MgB2 wires has been studied using Mg1-x PGMxB2 powders with low doping levels. It was found that Pt and Pd do not enter the MgB2 lattice and have only limited influence on Tc. In contrast, some Rh can be substituted and induces a decrease of Tc. Secondary phases are formed when the solubility limit is exceeded, but they have different morphologies depending on the dopant. For some of these PGM elements, flux pinning improvements have been observed at low fields. The results are discussed in comparison with previous investigations using other transition metals for doping on the Mg site.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ecosystems Programme, University of Barcelona
Authors: Grivel, J. (Intern), Alexiou, A. (Intern), Namazkar, S. (Intern), Pitillas, A. (Ekstern)
Number of pages: 5
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.395 SNIP 1.031
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.35 SNIP 0.935 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.364 SNIP 1.063 CiteScore 1.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.468 SNIP 1.073
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.452 SNIP 1.033
Web of Science (2009): Indexed yes
Effects of Biomass Feedstock on the Yield and Reactivity of Soot from Fast Pyrolysis at High Temperatures

This study investigated the effect of feedstock on the yield, nanostructure and reactivity of soot. Woody and herbaceous biomass were pyrolyzed at high heating rates and temperatures of 1250 and 1400°C in a drop tube furnace. The collected solid residues were structurally characterized by electron microscopy techniques, X-ray diffraction and N2-adsorption. The reactivity of soot was investigated by thermogravimetric analysis. The results showed that the reactivity of soot, generated at 1400°C was higher than that at 1250°C for all biomass types. Wood and wheat straw soot demonstrated differences with respect to the alkali content, particle size and nanostructure. Potassium was incorporated in the soot matrix and to a significant extent influenced the soot reactivity. The particle size distribution of pinewood soot produced at 1250°C was in the range from 27.2 to 263 nm which was broader compared to that of beechwood soot (from 33.2 to 102 nm) and wheat straw soot (from 11.5 to 165.3 nm). In addition, pinewood soot particles contained mainly multi-core structures at 1250°C. The potassium content played a more important role on the soot reactivity than the particle size and nanostructure.

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Main Research Area: Technical/natural sciences
Electronic versions:
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Effects of gas conditions on ASH induced agglomeration
Agglomeration is a serious problem for gasification and combustion of biomass in fluidized bed. Agglomeration characteristics may be affected by gas condition, but the literature is quite vague in this regard. This study focuses on the effects of gasification and combustion condition on agglomeration tendency with two types of biomass ash, including rice straw and wheat straw ash. The agglomerates are analyzed by SEM-EDS for morphology and elemental composition. Defluidization temperature (Td) in those two types of gas conditions is quite different. Td in gasification condition is much lower than that in combustion condition. Agglomeration in both combustion and gasification conditions are melting-induced, the lower Td gasification condition may be caused by the transformation of K2SO4.

General information
Effects of gasification biochar on plant-available water capacity and plant growth in two contrasting soil types

Abstract Gasification biochar (GB) contains recalcitrant carbon that can contribute to soil carbon sequestration and soil quality improvement. However, the impact of GB on plant-available water capacity (AWC) and plant growth in diverse soil types still needs to be explored. A pot experiment with spring barley (Hordeum vulgare L.) was conducted to investigate the effect of soil amendment by 1% straw and wood gasification biochar (SGB and WGB), respectively, on AWC and plant growth responses under two levels of water supply in a temperate sandy loam and a coarse sandy subsoil. In the sandy loam, the reduced water regime significantly affected plant growth and water consumption, whereas the effect was less pronounced in the coarse sand. Irrespective of the soil type, both GBs increased AWC by 17–42%, with the highest absolute effect in the coarse sand. The addition of SGB to coarse sand led to a substantial increase in plant biomass under both water regimes: shoot growth by 40–165% and root growth by 50–57%. However, no positive effects were achieved by the addition of WGB. In the sandy loam, soil application of GB had no or negative effects on plant growth. Our results suggest that SGB has considerable potential for enhancing crop productivity in coarse sandy soils by increasing soil water retention and improving root development.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Environmental Engineering, Roskilde University, University of Copenhagen
Authors: Hansen, V. (Forskerdatabase), Hauggaard-Nielsen, H. (Forskerdatabase), Petersen, C. T. (Forskerdatabase), Mikkelsen, T. N. (Intern), Müller-Stöver, D. S. (Forskerdatabase)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.74 SJR 1.353 SNIP 1.885
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.284 SNIP 1.877 CiteScore 3.08
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.669 SNIP 1.968 CiteScore 3.12
BFI (2013): BFI-level 1
Effects of several types of biomass fuels on the yield, nanostructure and reactivity of soot from fast pyrolysis at high temperatures

This study presents the effect of biomass origin on the yield, nanostructure and reactivity of soot. Soot was produced from wood and herbaceous biomass pyrolysis at high heating rates and at temperatures of 1250 and 1400 °C in a drop tube furnace. The structure of solid residues was characterized by electron microscopy techniques, X-ray diffraction and N2 adsorption. The reactivity of soot was investigated by thermogravimetric analysis. Results showed that soot generated at 1400 °C was more reactive than soot generated at 1250 °C for all biomass types. Pinewood, beechwood and wheat straw soot demonstrated differences in alkali content, particle size and nanostructure. Potassium was incorporated in the soot matrix and significantly influenced soot reactivity. Pinewood soot particles produced at 1250 °C had a broader particle size range (27.2–263 nm) compared to beechwood soot (33.2–102 nm) and wheat straw soot (11.5–165.3 nm), and contained mainly multi-core structures.
Effects of solid inertial particles on the velocity and temperature statistics of wall bounded turbulent flow

The effect of solid inertial particles on the velocity and temperature statistics of a non-isothermal turbulent channel flow is studied using direct numerical simulation. The particles inertia is varied by changing the particles diameter. The density of particles is kept constant. A two-way coupled Eulerian–Lagrangian approach is adopted to solve the carrier flow field and...
the motion of dispersed particles. Three different particle Stokes numbers of St = 24, 60, 192, at a constant particle mass loading of φm = 0.54, are considered. The mean and rms profiles of velocity and temperature for fluid and particles, and the scatter plots of fluid-particle temperature differences are presented. In addition, the variations of different budget terms for the turbulent kinetic energy equation and fluctuating temperature variance equation in the presence of particles are reported. The fluid turbulent heat flux is reduced by the presence of particles, and in spite of the additional heat exchange between the carrier fluid and the particles, the total heat transfer rate stays always lower for particle-laden flows. To further clarify this issue, the total Nusselt number is split into a turbulence contribution and a particle contribution, and the effects of particles inertia on fluid turbulent heat flux and fluid-particle heat transfer are examined in detail.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, South Dakota School of Mines & Technology
Authors: Nakhaei, M. (Intern), Lessani, B. (Ekstern)
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Scopus rating (2016): CiteScore 3.75 SJR 1.623 SNIP 2.005
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.797 SNIP 1.941 CiteScore 3.09
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.624 SNIP 2.008 CiteScore 2.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.868 SNIP 2.164 CiteScore 3.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.688 SNIP 2.17 CiteScore 2.79
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.085 SNIP 1.978 CiteScore 3.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.647 SNIP 2.12
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.712 SNIP 2.123
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.579 SNIP 1.957
Scopus rating (2007): SJR 1.76 SNIP 1.949
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.809 SNIP 1.962
Scopus rating (2005): SJR 1.818 SNIP 1.885
Scopus rating (2004): SJR 1.266 SNIP 1.918
Electrical Breakdown and Mechanical Ageing in Dielectric Elastomers

Dielectric elastomers (DE) are used in various applications, such as artificial eye lids, pressure sensors and human motion energy generators. For many applications, one of the major factors that limits the DE performance is premature electrical breakdown. There are many approaches that have been reported to increase the breakdown strength of DEs such as compositing and pre-stretching. Some of the techniques, however, affect other parameters related to DEs negatively. For instance, the elastomers with hard filler particles (e.g. metal oxides) used as DEs experience difficulties to maintain their long-term mechanical reliability as they are susceptible to Mullins effects as the results of pre-stretching. Therefore, two strategies are developed in this thesis in order to produce DEs with high electrical performance and long-term electromechanical reliability. The first strategy is to study the mechanisms behind the electrical breakdown of DEs and the second strategy is to investigate the long-term electromechanical reliability of DEs. In the first strategy, the electrothermal breakdown in polydimethylsiloxane (PDMS) elastomers was modelled in order to evaluate the thermal mechanisms behind the electrical failures. From the modelling based on the fitting of experimental data, it showed that the electrothermal breakdown of the PDMS elastomers was strongly influenced by the increase in both relative permittivity and conductivity. In addition to that, a methodology in determining the parameters that affect the breakdown strength of the pre-stretched DEs was developed. Breakdown strength was determined for samples with and without volume conservation and was found to depend strongly on the strain and the thickness of the samples.

In order for DEs to be fully implementable in commercial products, the lifetime of elastomer materials needs further investigation. Therefore, in the second strategy, several DE parameters such as Young's moduli, breakdown strengths and dielectric permittivities of PDMS elastomers filled with hard filler particles were investigated after being subjected to pre-stretching for various timespans. The study showed that electromechanical reliability when pre-stretching was difficult to achieve with PDMS elastomers filled with hard filler particles. Subsequently, the long-term mechanical and electrical reliability was further investigated to the PDMS elastomers filled with the soft fillers (e.g. oils). Interestingly, the results also showed that soft fillers significantly influence the long-term electromechanical reliability of PDMS elastomers. However, despite the pre-stretched PDMS elastomers filled with hard and soft filler experience difficulties to maintain their long-term electromechanical reliability, the study paves the way for electromechanically reliable DEs by indicating that simply post-curing PDMS elastomers before use.

Therefore in the last part of this thesis, the effect of post-curing was investigated for PDMS elastomer thin-films as a means of improving the long-term elastomer film electromechanical reliability. The PDMS elastomers were found to contain less than 2% of volatiles but nevertheless a strong effect from post-curing was observed. Furthermore, the determined electrical breakdown parameters from Weibull analyses showed that greater electrical reliability could be achieved by post-curing the PDMS elastomers before usage, and this method therefore paves a way towards more electromechanically reliable DEs.
Electrodialytic recovery of phosphorus from chemically precipitated sewage sludge ashes

Phosphorus scarcity requires improved recovery and reuse of urban sources; the recycling of this nutrient from sewage sludge has become increasingly important in the last years. Using an innovative electrodialytic process, the present study shows the potential for P separation from Fe and Al precipitated sewage sludge ash using this technique, with a recovery rate of around 70%. Furthermore, heavy metals were removed from the phosphorous fraction, producing a pure and safe phosphorus source in the end.

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Electrodialytic recovery of phosphorus from chemically precipitated sewage sludge ashes

Phosphorus scarcity requires improved recovery and reuse of urban sources; the recycling of this nutrient from sewage sludge has become increasingly important in the last years. Using an innovative electrodialytic process, the present study shows the potential for P separation from Fe and Al precipitated sewage sludge ash using this technique, with a recovery rate of around 70%. Furthermore, heavy metals were removed from the phosphorous fraction, producing a pure and safe phosphorus source in the end.

General information
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Energy recovery from water and food sector residual resources

General information
State: Published
Organisations: Department of Environmental Engineering, Residual Resource Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Pages: 64-72
Engineering model for intumescent coating behavior in a pilot-scale gas-fired furnace

In the event of a fire, intumescent fire protective coatings expand and form a thermally insulating char that protects the underlying substrate from heat and subsequent structural failure. The intumescence includes several rate phenomena, which have been investigated and quantified in the literature for several decades. However, various challenges still exist. The most important one concerns mathematical model validation under realistic exposure conditions and/or time scales. Another is the simplification of advanced models to overcome the often-seen lack of a complete set of input and adjustable model parameters for a given coating, thereby providing models for industrial applications. In this work, these two challenges are addressed. Three experimental series, with an intumescent coating inside a 0.65 m³ gas-fired furnace, were conducted and a very good repeatability was evident. The experiments were run for almost three hours, reaching a final gas temperature of about 1100 °C. Measurements include transient temperature developments inside the expanding char, at the steel substrate, and in the mineral wool insulation placed behind the substrate. A mathematical model, describing the intumescent coating behavior and temperatures in the furnace using a single overall reaction was developed and validated against experimental data. By including a decomposition front movement through the char, a good qualitative agreement was obtained. After further validation against experiments with other coating formulations, it has potential to become a practical engineering tool. This article is protected by copyright. All rights reserved.
Enhanced Oil Recovery with Application of Enzymes

Enzymes have recently been reported as effective enhanced oil recovery (EOR) agents. Both laboratory and field tests demonstrated significant increase in the ultimate oil production. Up to 16% of additional oil was produced in the laboratory conditions and up to 269 barrels of additional oil per day were recovered in the field applications. The following mechanisms were claimed to be responsible for the enhancement of the oil production due to enzymes: wettability improvement of the rock surface; formation of the emulsions; reduction of oil viscosity; and removal of high molecular weight paraffins. However, the positive effect of enzymes on oil recovery is not that obvious. In most of the studies commercial enzyme products composed of enzymes, surfactants and stabilisers were used. Application of such samples makes it difficult to assign a positive EOR effect to a certain compound, as several components of commercial mixture might possess surface-active properties. Hence, the main goals of the present study were to establish whether enzymes alone can improve oil production and to identify mechanisms that might underlie enzymatic EOR (EEOR), especially, under conditions of the North See petroleum reservoirs.

At the first stage of the work enzyme samples that might have potential for EOR applications were selected. Wettability tests such as measurements of contact angles and determination of adhesion behaviour were applied as screening tools.
The group of lipases/esterases demonstrated strong ability to detach oil from the calcite surface and was identified as the most promising group for further investigations. Wettability improvement due to protein adsorption on to the mineral was proposed as the main mechanism for EEOR. It was also proved that the enzyme molecules themselves caused change of the wetting state of calcite, while presence of stabilising ingredients did not interfere the results. Implementation of such a mechanism of enzymatic action under reservoir conditions might be limited by retention of the protein molecules in the porous medium. In order to verify this hypothesis, adsorption behaviour of enzymes/proteins on the reservoir rocks was studied by application of the static adhesion tests and adsorption experiments on powders, as well as of dynamic flow-through experiments. It was established that enzymes are indeed significantly lost during the transport in the porous media due to the irreversible adsorption. The adsorption capacity of carbonate material was found to be much higher compared to sandstone. Various methods (forexample, change of ionic strength and pH of the enzyme solution and displacing fluid) were applied in order to desorb attached protein molecules, but no desorption was observed. Another possible mechanism that might underlie EEOR is formation of enzyme-stabilised emulsions. Similar to the wettability screening, lipases/esterases demonstrated the best surface active properties: they formed the most stable emulsions with rather small drops. Light fractions of the crude oil participated mostly in formation of the protein-stabilised emulsions. Incubation of the oil-[enzyme + sea water] systems was found to be important in order to obtain high stability of emulsions. Combined application of enzymes and solid particles was an alternative way to increase emulsion stability. Other crude oil-brine interaction tests revealed additional problems that can rise during the application of enzymatic EOR. Interaction of the enzyme solution with the crude oil can induce gelation/emulsification of the propylene glycol (the main component of the enzyme productstabilisers). Moreover, when purified enzyme containing almost no stabilisers was used, a highly viscous oil-in-water emulsion was formed. Finally, assessment of enzymes as EOR agents under conditions similar to the conditions of the petroleum reservoirs was carried out in core flooding experiments. Two types of enzymes (lipase and amylase) were selected based on the results from the wettability and emulsion studies. They were only tested in tertiary mode, employing various injection schemes. Application of enzymes in sandstone core samples resulted in increase of the ultimate oil production by 0.23-1.69% relative to original oil in place, while no additional oil due to enzymes was produced from chalk. Wettability change was confirmed to be the main EOR mechanism, while emulsification plays less significant role. Overall, enzymes have possessed low potential for EOR applications at least in sandstone and chalk reservoirs containing light crude oils. An alternative technique that will shift adsorption balance towards reversible adsorption should be established in order to make enzymatic EOR an effective and economically feasible oil recovery method.

General information
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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Khusainova, A. (Intern), Shapiro, A. (Intern), Woodley, J. (Intern)
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Enhanced priming of old, not new soil carbon at elevated atmospheric CO₂
Rising atmospheric CO₂ concentrations accompanied by global warming and altered precipitation patterns calls for assessment of long-term effects of these global changes on carbon (C) dynamics in terrestrial ecosystems, as changes in net C exchange between soil and atmosphere will impact the atmospheric CO₂ concentration profoundly. In many ecosystems, including the heath/grassland system studied here, increased plant production at elevated CO₂ increase fresh C input from litter and root exudates to the soil and concurrently decrease soil N availability. Supply of labile C to the soil may accelerate the decomposition of soil organic C (SOC), a phenomenon termed ‘the priming effect’, and the priming effect is most pronounced at low soil N availability. Hence, we hypothesized that priming of SOC decomposition in response to labile C addition would increase in soil exposed to long-term elevated CO₂ exposure. Further, we hypothesized that long-term warming would enhance SOC priming rates, whereas drought would decrease the priming response. We incubated soil from a long-term, full-factorial climate change field experiment, with the factors elevated atmospheric CO₂ concentration, warming and prolonged summer drought with either labile C (sucrose) or water to assess the impact of labile C on SOC dynamics. We used sucrose with a 13C/12C signature that is distinct from that of the native SOC, which allowed us to assess the contribution of these two C sources to the CO₂ evolved. Sucrose induced priming of SOC, and the priming response was higher in soil exposed to long-term elevated CO₂ treatment. Drought tended to
decrease the priming response, whereas long-term warming did not affect the level of priming significantly. We were also able to assess whether SOC-derived primed C in elevated CO₂ soil was assimilated before or after the initiation of the CO₂ treatment 8 years prior to sampling, because CO₂ concentrations were raised by fumigating the experimental plots with pure CO₂ that was 13C-depleted compared to ambient CO₂. Surprisingly, we conclude that sucrose addition primed decomposition of relatively old SOC fractions, i.e. SOC assimilated more than 8 years before sampling.

**General information**

**State**: Published  
**Organisations**: Department of Chemical and Biochemical Engineering, University of Copenhagen, Lund University  
**Authors**: Vestergard, M. (Ekstern), Reinsch, S. (Intern), Bengtson, P. (Ekstern), Ambus, P. (Intern), Christensen, S. (Ekstern)  
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- Scopus rating (2016): SJR 2.132 SNIP 1.832 CiteScore 5.17  
- Web of Science (2016): Indexed yes  
- BFI (2015): BFI-level 2  
- Scopus rating (2015): SJR 2.305 SNIP 1.71 CiteScore 4.48  
- Web of Science (2015): Indexed yes  
- BFI (2014): BFI-level 2  
- Scopus rating (2014): SJR 2.349 SNIP 1.858 CiteScore 4.84  
- Web of Science (2014): Indexed yes  
- BFI (2013): BFI-level 2  
- Scopus rating (2013): SJR 2.271 SNIP 1.99 CiteScore 4.96  
- ISI indexed (2013): ISI indexed yes  
- Web of Science (2013): Indexed yes  
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- Scopus rating (2012): SJR 2.292 SNIP 1.74 CiteScore 4  
- ISI indexed (2012): ISI indexed yes  
- Web of Science (2012): Indexed yes  
- BFI (2011): BFI-level 2  
- Scopus rating (2011): SJR 2.146 SNIP 1.717 CiteScore 3.91  
- ISI indexed (2011): ISI indexed yes  
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- BFI (2010): BFI-level 2  
- Scopus rating (2010): SJR 1.868 SNIP 1.537  
- Web of Science (2010): Indexed yes  
- BFI (2009): BFI-level 2  
- Scopus rating (2009): SJR 2.044 SNIP 1.575  
- Web of Science (2009): Indexed yes  
- BFI (2008): BFI-level 2  
- Scopus rating (2008): SJR 1.955 SNIP 1.571  
- Web of Science (2008): Indexed yes  
- Scopus rating (2007): SJR 1.653 SNIP 1.567  
- Web of Science (2007): Indexed yes  
- Scopus rating (2006): SJR 1.896 SNIP 1.665
Entangled Polymer Melts in Extensional Flow

Many commercial materials derived from synthetic polymers exhibit a complex response under different processing operations such as fiber formation, injection moulding, film blowing, film casting or coatings. They can be processed both in the solid or in the melted state. Often they may contain two or more different polymers in addition to additives, fillers or solvents in order to modify the properties of the final product. Usually, it is also desired to improve the processability. For example the supplement of a high molecular weight component improves the stability in elongational flows. On the other hand, addition of low-volatility solvents to polymers is also a common industrial practice that others a means for lowering the Tg of the polymers. Moreover industrial polymers present a wide distribution of chain lengths and/or branched architectures that strongly influence their response.

Understanding the behaviour of polymer melts and solutions in complex non-linear flows is crucial for the design of polymeric materials and polymer processes. Through rheological characterization, in shear and extensional flow, of model polymer systems, i.e. narrow molar mass distribution polymer melts and solutions or well defined polymer molecules architecture, researchers develop constitutive equations that can relate the stress induced into a material with its flow deformation history. Indeed experiments on samples with well-defined structure supply data that can be compared with models.

Current models have been shown to be quite successful in describing the dynamics of polymers although they are still continuously challenged by new experimental data on model polymer systems. At the same time, new methods for generating extensional flows [McKinley and Sridhar (2002), Sentmanat (2004), Bach et al. (2003b)] are being constantly refined to improve the quality of the data and to explore a wider range of rates and deformations. Moreover, recently rheometry methods have been supplemented by other techniques such as dielectric spectroscopy that can probe chain dynamics and neutron scattering which can monitor macromolecular chain orientation associated with induced flow fields. This work concerns linear and non-linear rheology of polystyrene melts and solutions coupled with neutron scattering experiments. The aim of this thesis is to investigate the extensional properties of well characterized polymer samples and provide new experimental data on extensional rheology that can validate constitutive models. Moreover we show how the extensional technique may be used in combination with small-angle neutron scattering (SANS) to perform single chain structural studies after uniaxial elongation both after steady extensional flow and at several times during true stress relaxation. Extensional experiments have been performed on a Filament Stretching Rheometer (FSR), placed at the Technical University of Denmark (DTU), equipped with an online controlled scheme that allows to operate in controlled strain rate or controlled stress mode. High temperatures measurements can be performed due to an oven that surrounds the sample environment. Also a new implemented version of the device, named VADER 1000, has been employed to prepare the neutron scattering samples. The reduced dimension, compared to the FSR, and the particular design of the oven meets the requirement of fast cooling of the sample, so that it can freeze the particular molecular orientation of the chains at different stages of the stretching or relaxing of the sample.

General information

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Micro- and Nanotechnology, Amphiphilic Polymers in Biological Sensing
Authors: Hengeller, L. (Intern), Hassager, O. (Intern), Skov, A. L. (Intern), Almdal, K. (Intern)
Number of pages: 127
Entrained flow gasification of coal/bio-oil slurries

Coal/bio-oil slurry (CBS) is a new partial green fuel for bio-oil utilization. CBS reacts with gasification agents at high temperatures and converts into hydrogen and carbon monoxide. This paper provides a feasibility study for the gasification of CBS in an atmospheric entrained flow reactor for syngas production. Experiments have shown that CBS can be successfully processed and gasified in the entrained flow reactor to produce syngas with almost no tar content and low residual carbon formation. High reactor temperature and steam/carbon ratio is favourable for H2 production. At 1400 °C with steam/carbon ratio of 5, the syngas components are similar with that in equilibrium. A synergistic effect exists between coal and bio-oil in coal/bio-oil slurry gasification which might be caused by the catalysis effect of alkali metals and alkaline earth metals in bio-oil.
Entrained Flow Reactor Study of K-Capture by Solid Additives

A method to simulate the reaction between gaseous K-species and solid additives, at suspension fired conditions has been developed, using an entrained flow reactor (EFR). A water slurry containing solid additives (kaolin or coal fly ash) and KCl, is injected into the EFR and the solid products are collected from the cyclone and filter. The K-capture reaction is evaluated by determining the fraction of water-insoluble K in the products. The results showed that KCl can effectively be captured by kaolin and coal fly ash, forming water-insoluble K-aluminosilicates. The amount of K, captured per gram of additives, rose when increasing the molar ratio of K/(Al+Si) in the reactants. A change of the reaction temperature, from 1100 °C to 1450 °C, did not significantly influence the extent of the reaction, which is in contradiction to the trend observed in previous fixed-bed reactor studies. The method using the EFR, developed in this study, will be applied for further studies on the reaction of different additives and alkali species.

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**Entrained Flow Reactor Study of KCl Capture by Solid Additives**

An option for abating deposition and corrosion caused by alkali species during biomass combustion, is the introduction of additives into boilers for transforming harmful gaseous alkali compounds (e.g. KCl, KOH) into less corrosive ash species with a higher melting point. Kaolin and coal fly ash have been proved to be very promising additives and have received extensive studies during the past decades. However, most previous studies were carried out in fixed-bed reactors where the reaction conditions are obviously different from that in suspension-fired boilers. Detailed knowledge on the reaction between K-species and solid additives under suspension-fired conditions is still limited. In this study, a water slurry containing K-salt and solid additives was introduced into an entrained flow reactor (EFR) to study K-capture at suspension-fired conditions. A model will be developed based on experimental data and recommendations for optimal use of additives in full scale boilers will be provided.

**Environmental Assessment of Integrated Food and Cooking Fuel Production for a Village in Ghana**

Small-scale farming in Ghana is typically associated with synthetic fertilizer dependence and soil degradation. The farmers often rely on wood fuel for cooking imported from outside the farmland, a practice that is associated with deforestation. Integration of food and energy production may be a holistic approach to solving these issues. We study four approaches to providing food and fuel for cooking in a small-scale farming community. Present practice (PP) of synthetic fertilizer based food production and provision of wood fuel from outside the farming area is compared to three modeled, integrated technology options: integrated food and household-scale biogas production (HH Biogas), integrated food and village-scale biogas production (Village Biogas), and integrated food and wood fuel production (Agroforestry). Integrated approaches are able to eliminate the import of wood fuel, reduce synthetic fertilizer use by 24%, 35% and 44% and soil loss by 15%, 20% and 87%, respectively, compared to present practice. An Emergy Assessment (EmA) shows that integrated approaches are relevant substitutes to present practice considering biophysical efficiency indicated by Unit Emergy Value (in solar emjoules (sej) per J of output) and dependence on renewable inputs indicated by the Global Renewability Fraction (in %): 2.6–3.0 × 10^5 sej/J and 38%–48% (PP), 2.5–2.8 × 10^5 sej/J and 41%–46% (HH Biogas), 2.4–2.6 × 10^5 sej/J and 45%–47% (Village Biogas), 1.7–2.4 × 10^5 sej/J and 49%–66% (Agroforestry). Systematic recycling and use of local resources may play a pivotal role in reducing the dependence on non-renewable resources in Ghanaian farming, ensuring long-term soil fertility and stemming the current deforestation of wood reserves.

**General information**

**State:** Published

**Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, DONG Energy A/S

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**Publication information**

**Journal:** Sustainability
Environmental sustainability assessment of fruit cultivation and processing using fruit and cocoa residues for bioenergy and compost. Case study from Ghana

Agro-industrial businesses often have easy access to agricultural and processing residues with which they may reduce costs and pollution by integrating their production with bioenergy production. In regions with unreliable power supply, on-site electricity generation is a means to secure stable production conditions. Furthermore, recycling of nutrients may help to reduce biomass suppliers’ dependence on synthetic fertiliser. In this Environmental Sustainability Assessment (ESA) of fruit production in Ghana we compare two technology options for the production of mixed, fresh, tropical fruit, including cultivation, transport and processing. The option ‘Present practice’ presents data from a case study where production is characterised by soil loss and synthetic fertiliser dependence in cultivation and grid supply of electricity in processing. The option ‘Biogas’ is hypothetical and characterised by biogas and electricity production using farming and processing residues and by recycling of nutrients and carbon to soil. Cocoa shells are used as a co-substrate in the biogas production. Estimating the environmental impact of cocoa shell residues exposes the multifunctionality issue, continuously debated in ESA, particularly concerning bioenergy production. We compare the use of allocation of cocoa production impacts and system expansion that includes cocoa production as possible methods to manage multifunctionality of inputs. In assessments of residue-based production, we recommend using the latter method. Applying the system expansion method, we find that, in comparison with ‘Present practice’, the option ‘Biogas’ eliminates net soil carbon loss and reduces synthetic fertiliser, diesel and external electricity requirements at the expense of a relatively small increase in human labour input. The ESA includes the following indicators and shows that the ‘Biogas’ option is superior to ‘Present practice’ with regard to Cumulative Energy Demand (-39%), Cumulative fossil Energy Demand (-34%), Food Energy Return On energy Investment (þ65%), Food Energy Return On fossil energy Investment (þ53%) and Global Warming Potential (-29%) and similar to ‘Present practice’ in terms of the Emergy Assessment indicators Unit Emergy Value, Global Renewability Fraction, and Local Supply Fraction. Discarding the system expansion method, the same conclusion applies even if the emergy indicators are more ambiguous.
Environmental Sustainability Assessment of Integrated Food and Bioenergy Production with Case Studies from Ghana

The use of agricultural residues for the production of bioenergy offers tantalising prospects of reduced pollution and greater food sovereignty. Integrated food and bioenergy systems seek to optimise the joint production of food and energy. Integrated food and bioenergy systems may be evaluated and compared with other food and energy systems using Environmental Sustainability Assessment (ESA).

This thesis investigates a range of integrated food and residue-based bioenergy production systems and provide methodological developments that are relevant for the assessment of such systems. The methodological developments concern distribution of environmental burden in multifunctional systems; consistent accounting of human labour inputs; and modelling of uncertainty regarding future conditions. Residue-based bioenergy relies on feedstock from production systems that are multifunctional, which means that they provide several outputs. Environmental impact assessment of residue-based bioenergy, therefore, involves the identification of relevant impacts occurring prior to the conversion of residues into bioenergy. Dividing the environmental burden of food production between food and crop residues to maintain a single-product focus is a contentious practice, since no obvious allocation factor is available. In evaluations of bioenergy production systems that are based on residues from food production, it is recommended to expand the assessment’s system perspective to include food production and food outputs. Human labour is an indispensable input in all agricultural and bioenergy production activities evaluated in ESA. Assessment methods, however, differ with respect to accounting for human labour inputs. Emergy Assessment (EmA) routinely includes human labour inputs, but based on a variety of calculation approaches. The collection of methods referred to as LCA (Life Cycle Assessment) methods usually disregard human labour as a relevant input. It is suggested to adhere to a systematic approach to estimating the environmental impact of human labour inputs that is applicable in EmA and other ESAs. I recommend that human labour be accounted in labour time, and that labor’s environmental impact be based on all inputs required for making labour available.

Practices and technologies that are expected to be implemented several decades into the future and that are compared with existing alternatives should not solely be compared using current conditions. The evaluation of these systems must take into consideration that future conditions may be significantly different from current conditions. It is suggested to use explorative scenarios based on narratives of the future to emphasise and be transparent about the uncertainty involved with planning for the medium- to long-term. Modelling parameters may be deduced from such scenarios, making it possible to calculate scenario-dependent results. Applying the methodological developments above, two cases of integrated food and bioenergy production in Ghana are described. Crop residue-based biogas production and nutrient cycling in a remote village was shown to be a viable alternative to wood fuel and synthetic fertiliser use, in spite of increased labour inputs. In future scenarios where materials are scarce and labour plentiful, the investigated biogas-based and agroforestry technologies appear relatively more attractive. Fruit and cocoa residue-based biogas production in a fruit processing facility, with return of compost to pineapple farmers also proved to be a viable technology. It is recommended that relevant stakeholders explore the implementation of biogas and nutrient recycling technologies in preparation of reduced access to existing energy and nutrient sources. Primary contributions to the research field are suggested improvements to specific methods of evaluating integrated food and residue-based bioenergy systems. Evaluation of such systems requires an expanded system perspective that encompasses multiple outputs. It requires ways to properly account for labour, since energy and material input reductions, often associated with integration, result in increased labour inputs, as observed in the case studies. Evaluation also requires consideration of scenario uncertainty since implementation takes time and societal conditions may change significantly during the implementation phase. The contribution includes empirical data concerning farming and bioenergy conversion technologies in Ghana and a recommendation to implement biogas and nutrient recycling practices.
Enzymatic network for production of ether amines from alcohols

We constructed an enzymatic network composed of three different enzymes for the synthesis of valuable ether amines. The enzymatic reactions are interconnected to catalyze the oxidation and subsequent transamination of the substrate and to provide cofactor recycling. This allows production of the desired ether amines from the corresponding ether alcohols with inorganic ammonium as the only additional substrate. To examine conversion, individual and overall reaction equilibria were established. Using these data, it was found that the experimentally observed conversions of up to 60% observed for reactions containing 10mM alcohol and up to 280mM ammonia corresponded well to predicted conversions. The results indicate that efficient amination can be driven by high concentrations of ammonia and may require improving enzyme robustness for scale-up.

General information
State: Published
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.639 SNIP 1.366 CiteScore 4.04
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Enzymatic pretreatment of low-grade oils for biodiesel production

The alkaline process for making biodiesel (fatty acid methyl esters, or FAME) is highly efficient at the transesterification of glycerides. However, its performance is poor when it comes to using oil that contain significant amounts of free fatty acids (FFA). The traditional approach to such feed stocks is to employ acid catalysis, which is slow and requires a large excess of methanol, or to evaporate FFA and convert that in a separate process. An attractive option would be to convert the FFA in oil feedstocks to FAME, before introducing it into the alkaline process. The high selectivity of enzyme catalysis makes it a suitable basis for such a pretreatment process. In this work, we present a characterization of the pretreatment of high-FFA rapeseed oil using immobilized Candida antarctica lipase B (Novozym 435), focused on the impact of initial FFA and methanol concentration. Based on experimental results, we have identified limitations for the process in terms of FFA concentration in the feedstock and make suggestions for process operation. It was found that, using 5% catalyst and 4% methanol at 35°C, the FFA concentration could be reduced to 0.5% within an hour for feedstock containing up to 15% FFA. Further, the reaction was observed to be under kinetic control, in that the biocatalyst converts FFA (and FAME) at a much higher rate than glyceride substrates. There is thus, both a minimum and a maximum reaction time for the process to achieve the desired concentration of FFA. Finally, an assessment of process stability in a continuous packed bed system indicates that as much as 15m³ oil could potentially be pretreated by 1 kg of biocatalyst at the given process conditions.

General information
State: Published
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Enzyme Characterization in Microreactors by UV-Vis Spectroscopy

In protein engineering mutants are often selected solely on the basis of activity [1], simplifying the analysis and enabling high-throughput screening. At a later stage of development, several mutants show comparable performance and this basis for selection becomes indistinct. The basis for selection can at this point be improved by characterization of the enzyme performance where also inhibition and toxicity effects are taken into account. Enzyme characterization is here defined as the effect on initial rate of reaction with respect to pH, enzyme, substrate, co-substrate, product and co-product concentration [2]. From this investigation, it will be possible to determine whether the enzyme meets the criteria for process requirements or not. The development of the process will determine the requirements and this can also reach a state of maturity that resolves obstacles, lowers criteria and paves the way for implementation. As an example ω-transaminase is here investigated, which facilitates the exchange of an amine- and keto-group stereoselectively. The characterization will be carried out in a microreactor [3], this size is currently the only concept that can facilitate this thorough analysis, as the enzyme resource is scarce at this point of development. In the case where the reaction operates with UV active components, UV can be used to detect compounds with high sensitivity supplemented by multivariate data analysis. The spectra are here decorrelated and regressed to yield concentrations of individual compounds. HPLC systems are built for handling small quantities of liquids and the UV detectors for these proves to be fitting excellent. Enzyme characterization is therefore carried out by a combination of a microreactor with a diode array detector from an HPLC system.

General information
State: Published
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Number of pages: 1
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Enzyme discovery for fucoidan modification

General information
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Number of pages: 1
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Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

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Enzymes in CO2 Capture
The enzyme Carbonic Anhydrase (CA) can accelerate the absorption rate of CO2 into aqueous solutions by several-fold. It exist in almost all living organisms and catalyses different important processes like CO2 transport, respiration and the acid-base balances. A new technology in the field of carbon capture is the application of enzymes for acceleration of typically slow tertiary amines or inorganic carbonates. There is a hidden potential to revive currently infeasible amines which have an interesting low energy consumption for regeneration but too slow kinetics for viable CO2 capture. The aim of this work is to discuss the measurements of kinetic properties for CA promoted CO2 capture solvent systems. The development of a rate-based model for enzymes will be discussed showing the principles of implementation and the results on using a well-known tertiary amine for CO2 capture. Conclusions will be drawn revealing basic unexpected process conditions which are beneficial to enzyme promoted amines like water presence, temperatures, and similar basic variables.

General information
State: Published
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Main Research Area: Technical/natural sciences

Equation of State Selection for Organic Rankine Cycle Modeling Under Uncertainty
In recent years there has been a great interest in the design and selection of working fluids for low-temperature Organic Rankine Cycles (ORC), to efficiently produce electrical power from waste heat from chemical engineering applications, as well as from renewable energy sources such as biomass combustion, geothermal and solar heat sources. The working fluid is essential to the performance of the cycle. In order to evaluate and test promising fluid candidates, an appropriate Equation of State (EoS) [1] is necessary.

For ORC applications, an EoS is commonly selected based on goodness-of-fits to data, width of range of availability of fluid data and complexity of formulation, which is closely related to numerical expenses. We have explored an additional criterion for the selection of a particular EoS, namely the influence on the input uncertainty of the fluid parameters on the ORC model output.

We have recently presented a methodology [2] to propagate and quantify the impact of input property uncertainty and fluid property parameter uncertainty on the ORC model output. It is applied using different EoS: Cubic EoS such as Soave-Redlich-Kwong (SRK), Peng-Robinson (PR) and Perturbed Chain Statistical Association Fluid Theory (PC-SAFT). The different EoS are assessed based on the uncertainty propagated in the model output.

The study demonstrates that the range of property parameter uncertainty, the number of parameters, the sensitivity of the property parameter w.r.t to the EoS and the overall cycle, all influence the model output uncertainty.


General information
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Estimation of Kinetic Parameters in an Automotive SCR Catalyst Model
A challenge during the development of models for simulation of the automotive Selective Catalytic Reduction catalyst is the parameter estimation of the kinetic parameters, which can be time consuming and problematic. The parameter...
estimation is often carried out on small-scale reactor tests, or powder samples of the catalyst, which leads to problems when upscaling is done to the full-scale application. This contribution presents a methodology to sequentially estimate the kinetic parameters in 2 steps using steady-state limited small-scale reactor data, with the goal that the parameters should be used directly for accurate full-scale transient simulations. The model was validated against full-scale data with an engine following the European Transient Cycle. The validation showed that the predictive capability for nitrogen oxides (NOx) was satisfactory. After re-estimation of the adsorption and desorption parameters with full-scale transient data, the fit for both NOx and NH3-slip was satisfactory.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Haldor Topsoe AS
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Scopus rating (2013): SJR 1.125 SNIP 0.837 CiteScore 2.67
ISI indexed (2013): ISI indexed yes
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ISI indexed (2012): ISI indexed yes
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ISI indexed (2011): ISI indexed yes
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Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.269 SNIP 0.907
Web of Science (2009): Indexed yes
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Evaluation of the Cubic-Plus-Association Equation of State for Ternary, Quaternary, and Multicomponent Systems in the Presence of Monoethylene Glycol

Dew point specifications are of high interest in the natural gas industry. The CPA equation of state (EoS) was previously validated against both water content and phase equilibrium data. Moreover, solid model parameters were estimated for four natural gas main components (methane, ethane, propane, and carbon dioxide). In this study we have extended the use of CPA EoS to perform equilibrium temperature calculations for natural gas main components with (mono-)ethylene glycol (MEG) as an inhibitor. The ternary systems with aqueous MEG solution include methane, ethane, propane, carbon dioxide, and hydrogen sulfide. The quaternary systems with aqueous MEG solution include methane + ethane, methane + propane, methane + n-heptane, and methane + n-octane. Three multicomponent systems (>4 components) were also studied. The temperature range of the literature data is between 241.25–333.15 K, and the pressure range is between 0.1–24.8 MPa. The results in all cases are compared against experimental data, and very good agreement with experimental data is obtained.
Sulphur dioxide is well-known in the atmospheres of planets and satellites, where its presence is often associated with volcanism, and in circumstellar envelopes of young and evolved stars as well as the interstellar medium. This work presents a line list of 1.3 billion $^{32}$S$^{16}$O$_2$ vibration-rotation transitions computed using an empirically adjusted potential energy surface and an ab initio dipole moment surface. The list gives complete coverage up to 8000 cm$^{-1}$ (wavelengths longer than 1.25 μm) for temperatures below 2000 K. Infrared absorption cross-sections are recorded at 300 and 500 C are used to validated the resulting ExoAmes line list. The line list is made available in electronic form as supplementary data to this article and at www.exomol.com.
Sulphur trioxide (SO₃) is a trace species in the atmospheres of the Earth and Venus, as well as being an industrial product and an environmental pollutant. A variational line list for 32S¹⁶O₃, named UYT2, is presented containing 21 billion vibration-rotation transitions. UYT2 can be used to model infrared spectra of SO₃ at wavelengths longwards of 2 μm (ν < 5000 cm⁻¹) for temperatures up to 800 K. Infrared absorption cross-sections recorded at 300 and 500 C are used to validate the UYT2 line list. The intensities in UYT2 are scaled to match the measured cross-sections. The line list is made available in electronic form as supplementary data to this article and at www.exomol.com.
Experimental and Kinetic Modeling Study of C2H2 Oxidation at High Pressure

A detailed chemical kinetic model for oxidation of acetylene at intermediate temperatures and high pressure has been developed and evaluated experimentally. The rate coefficients for the reactions of C2H2 with HO2 and O2 were investigated, based on the recent analysis of the potential energy diagram for C2H3 + O2 by Goldsmith et al. and on new ab initio calculations, respectively. The C2H2 + HO2 reaction involves nine pressure- and temperature-dependent product channels, with formation of triplet CHCHO being dominant under most conditions. The barrier to reaction for C2H2 + O2 was found to be more than 50 kcal mol\(^{-1}\) and predictions of the initiation temperature were not sensitive to this reaction. Experiments were conducted with C2H2/O2 mixtures highly diluted in N2 in a high-pressure flow reactor at 600–900 K and 60 bar, varying the reaction stoichiometry from very lean to fuel-rich conditions. Model predictions were generally in satisfactory agreement with the experimental data. Under the investigated conditions, the oxidation pathways for C2H2 are more complex than those prevailing at higher temperatures and lower pressures. Acetylene is mostly consumed by recombination with H to form vinyl (reducing conditions) or with OH to form a CHCHO adduct (stoichiometric to lean conditions). Both C2H2 and CHCHO then react primarily with O2. The CHCHO + O2 reaction leads to formation of significant amounts of glyoxal (OCHCHO) and formic acid (HOCHO), and the oxidation chemistry of these intermediates is important for the overall reaction.
Experimental and Kinetic Modeling Study of Nitroethane Pyrolysis at a Low Pressure: Competition Reactions in the Primary Decomposition

The pyrolysis of nitroethane has been investigated over the temperature range of 682-1423 K in a plug flow reactor at a low pressure. The major species in the pyrolysis process have been identified and quantified using tunable synchrotron vacuum ultraviolet photoionization mass spectrometry and molecular beam sampling techniques. The rate constants for the primary pyrolysis of nitroethane as well as those for the decomposition of the secondary product CH$_3$CHNO$_2$ have been obtained via ab initio calculations. These results have been adopted in a detailed chemical kinetic model, which contains 95 species and 737 reactions. The model was validated against the experimental results with satisfactory agreement for most of the identified and quantified species. Further analysis on the results indicates that both the concerted molecular elimination and C-N bond rupture are significant in the primary pyrolysis of nitroethane, with the latter channel being more important at high temperatures. The adoption of new decomposition pathways of CH$_3$CHNO$_2$ has resulted in reasonable predictions for relevant intermediates.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Lawrence Livermore National Laboratory, University of Science and Technology of China, Shanghai Jiao Tong University, Centre National de la Recherche Scientifique
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Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
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Experimental investigation of a draft tube spouted bed for effects of geometric parameters on operation

Experiments are performed in a draft tube spouted bed (DTSB) to investigate effects of the operating conditions and the geometric parameters on the hydrodynamics. Geometry parameters, such as heights of the entrained zone, draft tube inner diameter, inner angle of the conical section were studied. Increasing the draft tube inner diameter, sharper inner angle of the conical section and higher height of entrained zone increase the internal solid circulation rate and the pressure drop. Even though, for all different configurations, higher gas feeding rate leads to higher internal solid circulation rate consideringa maximum value.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
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Scopus rating (2015): SJR 0.179 SNIP 0.217 CiteScore 0.18
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BFI (2013): BFI-level 1
Fouling-release coatings (FRC) were developed as an environmentally friendly alternative after the ban of highly toxic antifouling coatings based on tributyltin. Poly(dimethylsiloxane) (PDMS) has been the most widely used polymer for FRC, and its fouling-inhibition properties have been enhanced by addition of copolymers. Examples of these copolymers include phenyl-modified PDMS or poly(ethylene glycol) (PEG)-based copolymers (e.g. triblock PEG-b-PDMS-b-PEG). These copolymers diffuse from the bulk to the surface of the coating upon immersion and modify the physicochemical properties of the surface. FRC provide superior fuel savings to the shipping industry on the first stages of immersion compared to other current technologies, albeit its performance declines over time.

This project is mainly concerned with improving the understanding of FRC and identifying the causes that result in the worsening of the fouling-inhibition properties of these complex systems, specially focusing on the behaviour and fate of the block copolymers used as additives. The development of various methods to visualize and quantify processes involving these copolymers are presented. Chapter 1 provides an overview on marine biofouling, and the evolution and state-of-the-art in biofouling prevention. In Chapter 2, the scope, aims and hypotheses of this project are set. Chapter 3 studies the diffusion and biofouling-inhibition properties of PEG-based surfactants and copolymers added to PDMS and Chapter 4 analyses the distribution and behaviour of PEG-b-PDMS-b-PEG copolymers in PDMS coatings by fluorescence means. Chapter 5 investigates the degradation of PDMS-PEG-based copolymers in FRC immersed in seawater. Chapter 6 consists of a long-term field study regarding the release/loss of these block copolymers from fouling-release coatings. A coating based on a PDMS binder has been employed as model system in the thesis. The effect of the addition of various PEG-based surfactants and copolymers (i.e. amphiphiles) was investigated by a novel method developed in this project, and the diffusion coefficient and biofouling-inhibition properties of the different amphiphiles were studied. The results showed that there is a moderate dependence of the diffusion coefficient on the molecular weight of the molecule. The diffusion coefficients obtained were relatively high for all the investigated compounds with molecular weights (Mw) ranging from 600 to 4000 g/mol. Moreover, the biofouling-inhibition properties are not dependant on the diffusion coefficient of the amphiphiles, but mainly depend on the chemistry of the hydrophobic block, with PDMS-PEG-based copolymers providing the best results. Hence, the anchoring capabilities and stability of the copolymer on the surface of the coating are proven to be a central aspect of the performance of these FRC.

A novel fluorescent-labelled triblock PEG-b-PDMS-b-PEG copolymer was synthesized in this project to visualize the
distribution and behaviour of PDMS-PEG-based copolymers in PDMS coatings. Images obtained by confocal microscopy proved that the copolymer molecules assemble in spherical domains inside the PDMS coating. The domains are smaller close to the surface and larger in the bulk of the film (with domains as large as 7 μm in diameter). The diffusion of copolymer from the bulk to the interfaces of the PDMS film could be observed by following the fluorescence intensity at different depths over time.

The chemical stability of PDMS-PEG-based copolymers in PDMS coatings immersed for up to 30 months in seawater in Singapore was also investigated. The copolymer remaining in the coatings after exposure was extracted and isolated, and its chemical composition was analysed. An increase in the relative content of PDMS was observed, probably due to the imperfect isolation process. However, no traces of degradation products were found, and it was observed that the molecular weight of the copolymer did not change over time. Therefore, it was concluded that the copolymer molecules remaining in the coating after 30 months of immersion did not suffer significant degradation. Conversely, the studied copolymers could be degraded in the laboratory under a range of conditions and the degradation products were successfully identified, mainly consisting of esters arising from the oxidative degradation of the PEG block. Further experiments showed that degradation can also occur in the bulk of the coatings depending on the physical properties and chemical composition of some of the constituents of FRC, both for coatings immersed in seawater and others kept in the laboratory in dry conditions.

The release/loss of copolymer from FRC was also studied, and the effect of different variables such as seawater temperature and the addition of biocide were addressed. Approximately 300 experimental coatings exposed to seawater for up to 5 years were analysed and the results exhibited a large scatter in the data, mainly attributed to differences in the coatings compositions. However, some comparable formulations suggest that seawater temperature has an important effect on the loss of copolymer from PDMS-coatings, while the initial concentration of copolymer has no influence for copolymer concentrations as high as 7 wt%. In addition, the initial concentration of biocide showed diverse effects, with biocide-containing coatings leading to higher copolymer losses in the first stages of immersion and larger copolymer retention values in long-term exposure, indicating that the addition of biocide strongly influences the release profile of these copolymers from FRC.

In summary, the addition of block copolymers is a successful method to impart biofouling-inhibition properties to fouling-release coatings. The development of new methodologies has allowed the investigation of the behaviour and fate of these block copolymers in FRC. While the performance of these copolymers is not limited by its diffusion properties in the film, attention should be put on the physical properties and chemical composition of the copolymer and other coating constituents. These variables have an important influence on the anchoring, release and degradation of these copolymers, which dictate the long-term performance of fouling-release coatings.

**General information**

State: Published  
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**Relations**

Projects: Experimental investigation of the behaviour and fate of block copolymers in fouling-release coatings  
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**Experimental investigations and modeling of devolatilization based on superimposed kinetics of biomass**

A non-isothermal one-dimensional model has been developed to describe biomass pyrolysis at fast heating rate \( (600-10^4 \text{ Ks}^{-1}) \), high temperatures \( (up to 1500^\circ C) \) and is valid for different biomass particle sizes \( (< 10 \text{ mm}) \). The model was developed to estimate the yields of volatile gas and char. The model relies on the concept applied in fast pyrolysis of cellulose through the formation of an intermediate liquid (so called metaplast) which reacts further to char and gas. The kinetics of the fastpyrolysis was described by the Broido-Shafizadeh scheme. The influence of particle size and shape was included in the model. Cylindrical representation of a biomass particle shape was chosen to be the most suitable in the pyrolysis model. The evolution of devolatilization time required for the complete pyrolysis showed that the particles with a mean diameter \(< 0.45\text{mm} \) may be considered as thermally thin at high heatingrates. The predicted results by one-dimensional model are in agreement with the experimental work, and emphasize a keyrole of intra-particle heat conduction in biomass particles > 0.45 mm. The potassium influence on the char yield was implemented in the model based on the experimental results in the wire meshand drop tube reactors with respect to the stronger catalytic effect of potassium on the char yield at low and intermediate heating rates compared to pyrolysis at high heating rates. The heating
rate and potassium content affected significantly the char yield as evidenced from the experimental data obtained in the wire mesh and drop tube reactors. Thus, the model including these two parameters provides an acceptable fit of char yield to the experimental data. The present results showed that the proposed kinetic model for the fast biomass pyrolysis is relatively simple and predicts reasonably accurately the char yield of woody and herbaceous biomass particles < 10mm using one fixed set of kinetic parameters valid for woody and herbaceous biomass.

General information
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Authors: Trubetskaya, A. (Intern), Jensen, A. D. (Intern)
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Extension of apparent devolatilization kinetics from thermally thin to thermally thick particles in zero dimensions for woody biomass
This work aims to provide an accurate and simple model, predicting the time dependent devolatilization of woody biomass at conditions (Tgas < 2000 K) and particle sizes (<2 mm) relevant to suspension fired boilers. The zero dimensional model is developed from reference calculations with a one-dimensional heat transport model coupled with a drying and a devolatilization model. The model output has been used to generate pyrolysis kinetics corrected for non-isothermal effects, i.e. intraparticle heat transport limitations. Analysis of the modeling results indicate that heat transport corrections of even small particles are necessary. The current work divides a given particle size distribution into suitable size categories based on their internal heat transport properties. The devolatilization is described by size category specific rate constants based on a single first order reaction mechanism. This approach allows for significantly more accurate devolatilization predictions of any particle size distribution to be described by simple kinetic mechanisms and isothermal particle heat balances. Such an approach is easily implemented into most commercial CFD (computational fluid dynamics) codes without adding any additional strain to the computational requirements.

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Fabrication of scalable tissue engineering scaffolds with dual-pore microarchitecture by combining 3D printing and particle leaching

Limitations in controlling scaffold architecture using traditional fabrication techniques are a problem when constructing engineered tissues/organs. Recently, integration of two pore architectures to generate dual-pore scaffolds with tailored physical properties has attracted wide attention in tissue engineering community. Such scaffolds features primary structured pores which can efficiently enhance nutrient/oxygen supply to the surrounding, in combination with secondary random pores, which give high surface area for cell adhesion and proliferation. Here, we present a new technique to fabricate dual-pore scaffolds for various tissue engineering applications where 3D printing of poly(vinyl alcohol) (PVA) mould is combined with salt leaching process. In this technique the sacrificial PVA mould, determining the structured pore architecture, was filled with salt crystals to define the random pore regions of the scaffold. After crosslinking the casted polymer the combined PVA-salt mould was dissolved in water. The technique has advantages over previously reported ones, such as automated assembly of the sacrificial mould, and precise control over pore architecture/dimensions by 3D printing parameters. In this study, polydimethylsiloxane and biodegradable poly(-caprolactone) were used for fabrication. However, we show that this technique is also suitable for other biocompatible/biodegradable polymers. Various physical and mechanical properties of the dual-pore scaffolds were compared with control scaffolds with either only
structured or only random pores, fabricated using previously reported methods. The fabricated dual-pore scaffolds supported high cell density, due to the random pores, in combination with uniform cell distribution throughout the scaffold, and higher cell proliferation and viability due to efficient nutrient/oxygen transport through the structured pores. In conclusion, the described fabrication technique is rapid, inexpensive, scalable, and compatible with different polymers, making it suitable for engineering various large scale organs/tissues.

Factors Contributing to Activity in Catalytic Soot Oxidation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics, CHEC Research Centre
Fast pyrolysis of biomass at high temperatures

This Ph.D. thesis describes experimental and modeling investigations of fast high temperature pyrolysis of biomass. Suspension firing of biomass is widely used for power generation and has been considered as an important step in reduction of greenhouse gas emissions by using less fossil fuels. Fast pyrolysis at high temperatures plays a significant role in the overall combustion process since the biomass type, the reaction kinetics and heat transfer rates during pyrolysis influence the volatile gas release. The solid residue yield and its properties in suspension firing, including particle size and shape, composition, reactivity and burnout depend significantly on the operating conditions of the fast pyrolysis. Biomass fast pyrolysis experiments were performed in a laboratory-scale wire mesh reactor and bench scale atmospheric pressure drop tube / entrained flow reactors with the aim to investigate the effects of operating parameters and biomass types on yields of char and soot, their chemistry and morphology as well as their reactivity using thermogravimetric analysis. The experimental study was focused on the influence of a wide range of operating parameters including heat treatment temperature, heating rate, particle size, residence time, inorganic matter and major organic biomass compounds. Woody and herbaceous biomass were used as fuels. Char yields from the drop tube and entrained flow reactors were lower than those obtained in the wire mesh reactor, emphasizing the importance of heat transfer on the product yields. The char yield decreased significantly between 10 and 600K s⁻¹, but continued to decrease with increasing heating rate, and was lowest for the drop tube / entrained flow reactors with estimated heating rate of > 10⁶ K s⁻¹. The heat treatment temperature and potassium content affected the char yield stronger than the heating rates and differences in the plant cell wall compounds between 600 and 3000K s⁻¹. The heat treatment temperature affected more the herbaceous biomass char yield compared with wood.

The differences in the char yield for particle size fractions in the range of 0.05mm were negligible, leading to the conclusion that the biomass particle can be assumed isothermal, when its size did not exceed 0.425 mm. Compared to smaller particles, the larger pinewood particles (d₅₀ > 0.85 mm) required more than 1 s holding time for the complete conversion in intermediate fast heating rates. The influence of heating rate on the char yields was less pronounced for hardwood charcoal, with a 1.5 to 2.5 fold increase from 0.85 to 4 mm in temperature at temperatures > 1250°C in the wire mesh reactor, single particle burner and drop tube reactor, due to the predominance of internal heat transfer control within the large particles.

Potassium compared to all other ash elements in the fuels had the highest influence on the char yield. The effect of potassium on the char yield was stronger at low and intermediate heating rates where potassium catalyzed the repolymerization and cross-linking reactions, leading to higher char yields. Silicon compounds abundant in herbaceous biomass had a negligible influence on the char yield and reactivity. However, a very high content of silicon oxides in biomass (> 50% of the overall biomass inorganic matter) significantly affected the char morphology, as observed for rice husk. For this fuel, the high content of low-temperature melting amorphous silicon oxides led to the formation of a glassy shell on rice husk chars at 1000-1500°C. The ability of char to melt in fast pyrolysis followed the order pine > beechwood, straw > rice husk, and was related to the formation of metaplast. Different particle shapes of beechwood and leached wheat straw chars produced in the drop tube reactor which have similar potassium content suggested a stronger influence of the major biomass cell wall compounds (cellulose, hemicellulose, lignin and extractives) and silicates on the char morphology than alkali metals. In this study, potassium lean pinewood (0.06 wt. %) produced the highest soot yield (9 and 7 wt. %) at 1250 and 1400°C, whereas leached wheat straw with the higher potassium content (0.3 wt. %) generated the lowest soot yield (2 and 1 wt. %). Soot yields of wheat and alfalfa straw at both temperatures were 5% points lower than wood soot yields and 3% points higher than leached wheatstraw soot yield, indicating that potassium plays a minor role on the soot formation. The leaching of alkali from wheat straw additionally resulted in a removal of lignin, leading to the decreased formation of polycyclic aromatic hydrocarbon precursors, and thereby to lower soot yields. Pinewood soot particles generated at 1250°C were significantly larger (77.7 nm) than soot particles produced in pinewood (47.8 nm) pyrolysis at 1400°C, beechwood (43 nm) and wheat straw (30.8 nm) devolatilization at both temperatures. The larger pinewood soot particles were related to the formation of tar balls known from smoldering combustion. The major difference in nanostructure of pinewood, beechwood and wheat straw chars at 1000-1500°C was related to the formation of tar balls known from smoldering combustion. Different particle shapes of beechwood and rice husk chars at 1000-1500°C. The ability of char to melt in fast pyrolysis followed the order pinewood > rice husk > beechwood, straw > rice husk, and was related to the formation of metaplast. Different particle shapes of beechwood and leached wheat straw chars produced in the drop tube reactor which have similar potassium content suggested a stronger influence of the major biomass cell wall compounds (cellulose, hemicellulose, lignin and extractives) and silicates on the char morphology than alkali metals. In this study, potassium lean pinewood (0.06 wt. %) produced the highest soot yield (9 and 7 wt. %) at 1250 and 1400°C, whereas leached wheat straw with the higher potassium content (0.3 wt. %) generated the lowest soot yield (2 and 1 wt. %). Soot yields of wheat and alfalfa straw at both temperatures were 5% points lower than wood soot yields and 3% points higher than leached wheatstraw soot yield, indicating that potassium plays a minor role on the soot formation. The leaching of alkali from wheat straw additionally resulted in a removal of lignin, leading to the decreased formation of polycyclic aromatic hydrocarbon precursors, and thereby to lower soot yields. Pinewood soot particles generated at 1250°C were significantly larger (77.7 nm) than soot particles produced in pinewood (47.8 nm) pyrolysis at 1400°C, beechwood (43 nm) and wheat straw (30.8 nm) devolatilization at both temperatures. The larger pinewood soot particles were related to the formation of tar balls known from smoldering combustion. The major difference in nanostructure of pinewood, beechwood and wheat straw soot was in the formation of multi and single core particles. Pinewood soot particles generated at 1250°C were mainly multi core structures compared to pinewood soot generated at 1400°C, combining both single and multi core particles. Beechwood and wheat straw soot samples had multi and single core particles at both temperatures. In thermogravimetric analysis, the maximal reaction rate of pinewood soot was shifted to temperatures about 100°C higher than for the other samples in both oxidation and CO₂ gasification, indicating a significantly lower reactivity. Soot samples produced at 1400°C were more reactive than soot generated at 1250°C. The beechwood and wheat straw soot samples were more graphitic than pinewood soot based on the electron energy loss spectroscopy (EELS) analysis. In contrast to expectations of graphitic structures to react slower than amorphous samples, beechwood and wheat straw soot were 35 and 571 times more reactive than pinewood soot prepared at 1400°C. The presence of potassium in wheat straw soot mainly as water-soluble KCl, KOH, KHCO₃ and K₂CO₃ and to a minor extent bonded to the soot matrix in oxygen-containing surface groups (e.g., carboxyl, phenolate) or intercalated in soot graphene layers led to a higher reactivity in CO₂ gasification compared to low-alkali containing pinewood soot. The results showed that potassium has a dominating effect on the soot reactivity compared to nanostructure and particle size. A mathematical
model of biomass fast pyrolysis was developed to predict the gas and char yield of wood and herbaceous biomass at heating rates $> 600\text{K s}^{-1}$. The model includes both kinetics and external and internal heat transfer assuming that mass transfer is fast. The model relies on the concept applied in fast pyrolysis of cellulose through the formation of an intermediate liquid (socalled metaplast) which reacts further to form char and gas. The kinetics of the fast pyrolysis was described through the Broido-Shafizadeh scheme for biomass. The catalytic effect of potassium which is a major ash element influencing the char yield was included in the model.

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Fast pyrolysis of biomass at high temperatures
Publication: Research › Ph.D. thesis – Annual report year: 2016

Final report V1.0 for the CORE Organic II funded project: Coordinating Organic Breeding Activities for Diversity - COBRA
Post project summary suitable for web publication
Background
Plant breeding is crucial in creating organic crop production systems that can better cope with interacting stresses such as pests and diseases (especially seed-borne diseases), weeds and the increasingly erratic and unpredictable variation in climate and weather. In this context, COBRA aimed to support and develop organic plant breeding and seed production with a focus on increasing the use and potential of plant material with high genetic diversity in cereals (wheat and barley) and grain legumes (pea and faba bean), through coordinating, linking and expanding existing breeding and research. Although systems based on high, within-crop diversity have shown promising results in organic systems and are now subject to intensive research, their benefits cannot be exploited currently, due to agronomic, regulatory and other hurdles. Also, it is currently unclear which plant breeding approaches, high diversity or otherwise, are most efficient to breed varieties for organic agriculture. To help these aims, COBRA's work was arranged into a management workpackage to coordinate the work and the following five sub-programmes:

(1) To improve methods ensuring seed quality and health
Progress was made in handling individual seeds in terms of their actual and potential resistance to seed-borne disease. One of the most important problems, bunt of wheat, was advanced considerably in terms of the 'gene for gene' interaction between host and pathogen and in observing the performance of the, currently, most effective resistance genes. Wheat populations, grown over two generations, did not change in their response to bunt. In barley, progress was made in identifying and confirming known and novel resistances to a range of the most important seed-borne diseases. Benign sprays were confirmed as potentially useful for Ascochyta blight control in peas.

(2) To determine the potential to increase resilience, adaptability, and overall performance in organic systems by using crop diversity at various levels
Valuable progress was made in confirming, expanding and understanding the resilience of the performance of composite cross populations of wheat. A wide range of molecular markers were identified in barley which will help in selecting genotypes adapted to expected future changes in climate and weather. Progress was also made with organic trials of grain legumes. The early 6 of 54 development stages of composite cross populations in the field is now better understood in relation to nutrient use efficiency.

(3) To improve breeding efficiency and to develop novel breeding methods to enhance and maintain crop diversity
A range of different technologies has been improved for selecting within composite cross populations using NIR spectrometry, colour markers and molecular markers; many of these are non-destructive. Of more immediate value, new composite cross populations involving winter and spring wheat genotypes and including bunt resistant genotypes have now been made. Progress has also been made with bulk breeding of peas, although single genotypes may still be preferred for cropping applications.

(4) To identify and remove structural barriers to organic plant breeding and seed production
It was important to bring together interested individuals and groups from different European countries to cover available experience and discuss further developments. Most importantly, this was also done directly in consultation with DGSanco, and booklets on the discussions and findings were published and distributed.
To improve networking and dissemination in organic plant breeding, COBRA successfully established and utilised its website, produced regular newsletters and undertook training and farm days throughout the life of the project to raise the awareness of the project and to also communicate and discuss the finds and outcomes of the work undertaken by its various partners.

Conclusion.

COBRA’s strength is its focus on coordinating, linking and expanding ongoing organic breeding activities in cereals and grain legumes across Europe, drawing together experts from previously separated areas.

General information

State: Published
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Forbedring af industrielle processes energieffektivitet

Et dansk forskningsprojekt, THERMCYC, arbejder på at udvikle løsninger, som kan gøre udnyttelsen af overskudsvarme til el- og varmeproduktion økonomisk og teknisk mulig og dermed øge industriens bæredygtighed.

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Forbedring af industrielle processes energieffektivitet

Et dansk forskningsprojekt, THERMCYC, arbejder på at udvikle løsninger, som kan gøre udnyttelsen af overskudsvarme til el- og varmeproduktion økonomisk og teknisk mulig og dermed øge industriens bæredygtighed.

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Formation of water-soluble soybean polysaccharides from spent flakes by hydrogen peroxide treatment

In this paper we propose a novel chemical process for the generation of water-soluble polysaccharides from soy spent flake, a by-product of the soy food industry. This process entails treatment of spent flake with hydrogen peroxide at an elevated temperature, resulting in the release of more than 70% of the original insoluble material as high molar mass soluble polysaccharides. A design of experiment was used to quantify the effects of pH, reaction time, and hydrogen peroxide concentration on the reaction yield, average molar mass, and free monosaccharides generated. The resulting product is low in protein, fat, and minerals and contains predominantly water-soluble polysaccharides of high molar mass, including arabinan, type I arabinogalactan, homogalacturonan, xyloglucan, rhamnogalacturonan, and (glucurono)arabinoxylan. This treatment provides a straightforward approach for generation of soluble soy polysaccharides and opens a new range of opportunities for this abundant and underutilized material in future research and industrial applications.
From a single pellet press to a bench scale pellet mill - Pelletizing six different biomass feedstocks

The increasing demand for biomass pellets requires the investigation of alternative raw materials for pelletization. In the present paper, the pelletization process of fescue, alfalfa, sorghum, triticale, miscanthus and willow is studied to determine if results obtained in a single pellet press (SPP) can be extrapolated to larger scale pellet mills. The single pellet press was used to find the optimum moisture content and die operating temperature for pellet production. Then, these results were compared with those obtained from a bench-scale pellet mill. A moisture content of around 10 wt.% was found to be optimal for the six biomass feedstocks. A friction increase was seen when the die temperature increased from room temperature to 60-90 degrees C for most biomass types, and then a friction decrease when the die temperature increased further. The results obtained in the bench-scale pellet mill support the proposed theory that good quality pellets and satisfactory pelletizing should occur in the region where the friction decreases with die temperature. Therefore, the friction vs. die temperature curve measured for each biomass in the SPP can be used as an indication of the right die temperature in large-scale pellet production. (C) 2015 Elsevier B.V. All rights reserved.
Fuel Quality Impact in a Historical Perspective: A Review of 25 Years of EU-Funded Research on Fuel Characterization, Ash and Deposit Formation, and Corrosion

Heating and cooling are responsible for approximately half of EU’s final energy demand, while biomass is currently responsible for more than 90% of all renewable heat. The goal is to increase share of biomass-based technologies, in the European heat market, from 11% in 2007 to about 25% in 2020 [RHC-Platform, 2014]. Combined Heat and Power (CHP) from biomass is a suitable technology for medium- and large scale units, where many utility and industrial applications can be found, especially in Scandinavia. The main challenge for efficient CHP and high temperature steam production from biomass are ash-related problems. Corrosion due to the difficult ash composition of biomass limits both steam temperature and efficiency. By solving these issues, large-scale boilers offer a huge potential for efficiency increase and emission reduction, during CHP generation at cost-competitive and environmental friendly conditions. In order to reach these goals, and to enable a secure and nearly carbon neutral heat and power generation, recently, the Biofficiency proposal, was granted under Horizon2020, aiming to:

Develop next generation, biomass-fired CHP plant, increasing the steam temperatures up to 600°C, at medium to large scale (10 to 200 MWth).

Increase the efficiency of CHP plants by elevated steam temperatures through solving and understanding of ash-related problems – slagging, fouling and corrosion.

Reduce emissions – i.e. CO2, particulates, CO, NOX, and SO2 – by efficiency gain, reduction of impurities and by intelligent plant design.

Broaden the feedstocks for pulverized fuel (PF) and fluidized bed (FB) powerplants, using pre-treatment methods with focus on the reduction of harmful, inorganic elements: Cl, S and the alkali metals.

Prevent power plant damage due to high-temperature Cl-induced corrosion.

Reduce costs for utilities due to increased efficiency, lowered emissions and fuel consumption, decreased number of outages and maintenance due to handling of ash-related problems.

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Functional bio-based polyesters by enzymatic polymerization
During recent years enzymatic polymerization has become increasingly popular as an alternative to classical polyesterification processes. The high regioselectivity observed for lipases permits preparation of novel polyesters with a high number of functional groups. 1 This is particularly interesting when considering monomers from bio-based feedstock that generally contain a high number of functional groups such as both secondary and primary alcohols. Enzymatic polymerization can be conducted at relatively low temperature and thereby is well suited for sensitive monomers. Recently enzymatic polymerization was applied to prepare functional water soluble polyesters based on dimethyl itaconate and poly(ethylene glycol).2 The monomer permits postfunctionalization using thiol-ene chemistry or aza-michael additions, which was used to illustrate the possibilities of preparing functional hydrogels. Hydrogels based on the polyesters were shown to be degradable and could be prepared either from the pure polyester or from prefunctionalized polyesters, though the thiol-ene reactions were found to be less effective. Since then a new monomer, trans,2,5-dihydroxy-3-pentenoic acid methyl ester (DPM) has been prepared directly from pentoses using using tin containing zeolites.3 The monomer was prepared in yields of up to 32% and contains both a vinyl as well as a secondary alcohol in addition to the primary alcohol and ester functionality, and as such is an interesting building block for polymers. DPM was copolymerized together with ethyl-6-hydroxyhexanoate yielding copolymers with molecular weights of up to 12,000 g/mol. The polymers were postfunctionalized using trifluoroacetic anhydride, which resulted in 100% conversion of the secondary alcohols, illustrating the possibility to use the secondary alcohol for grafting. In addition to this, thiol-ene reactions using hexanethiol, mercaptoethanol, mercaptoacetic acid, 2-ethylhexanethiol and thiophenol were conducted on the internal double bond resulting in conversions of 32-100%. Given the lower reactivity of the internal double bond the extent of functionalization was found acceptable for use as a general method for dual functionality polyesters.
Functional Unfold Principal Component Regression Methodology for Analysis of Industrial Batch Process Data

This work proposes a methodology utilizing functional unfold principal component regression (FUPCR), for application to industrial batch process data as a process modeling and optimization tool. The methodology is applied to an industrial fermentation dataset, containing 30 batches of a production process operating at Novozymes A/S. Following the FUPCR methodology, the final product concentration could be predicted with an average prediction error of 7.4%. Multiple iterations of preprocessing were applied by implementing the methodology to identify the best data handling methods for the model. It is shown that application of functional data analysis and the choice of variance scaling method have the greatest impact on the prediction accuracy. Considering the vast amount of batch process data continuously generated in industry, this methodology can potentially contribute as a tool to identify desirable process operating conditions from complex industrial datasets. © 2016 American Institute of Chemical Engineers AIChE J, 2016
This chapter gives an overview of the fundamentals of process intensification from a process systems engineering point of view. The concept of process intensification, including process integration, is explained together with the drivers for applying process intensification, which can be achieved at different scales of size, that is, the unit operation scale, the task scale, and the phenomena scale. The roles of process intensification with respect to process improvements and the generation of more sustainable process designs are discussed and questions related to when to apply process intensification and how to apply process intensification are answered through illustrative examples. The main issues and needs for generation of more sustainable process alternatives through process intensification are discussed in terms of the need for a systematic computer-aided framework and the methods and tools that should be employed through it. The process for the production of methyl-acetate is used as an example to highlight the generation of more sustainable process alternatives through this framework. Perspectives, conclusions, and future work are proposed in order to further develop the field of process intensification using a systems approach.
Fusion characterization of biomass ash

The ash fusion characteristics are important parameters for thermochemical utilization of biomass. In this research, a method for measuring the fusion characteristics of biomass ash by Thermo-mechanical Analyzer, TMA, is described. The typical TMA shrinking ratio curve can be divided into two stages, which are closely related to ash melting behaviors. Several characteristics temperatures based on the TMA curves are used to assess the ash fusion characteristics. A new characteristics temperature, $T_m$, is proposed to represent the severe melting temperature of biomass ash. The fusion characteristics of six types of biomass ash have been measured by TMA. Compared with standard ash fusibility temperatures (AFT) test, TMA is more suitable for measuring the fusion characteristics of biomass ash. The glassy molten areas of the ash samples are sticky and mainly consist of K-Ca-silicates.
The use of process models to simulate the fate of micropollutants in wastewater treatment plants is constantly growing. However, due to the high workload and cost of measuring campaigns, many simulation studies lack sufficiently long time series representing realistic wastewater influent dynamics. In this paper, the feasibility of the Benchmark Simulation Model No. 2 (BSM2) influent generator is tested to create realistic dynamic influent (micro)pollutant disturbance scenarios. The presented set of models is adjusted to describe the occurrence of three pharmaceutical compounds and one of each of its metabolites with samples taken every 2-4h: the anti-inflammatory drug ibuprofen (IBU), the antibiotic sulfamethoxazole (SMX) and the psychoactive carbamazepine (CMZ). Information about type of excretion and total consumption rates forms the basis for creating the data-defined profiles used to generate the dynamic time series. In addition, the traditional influent characteristics such as flow rate, ammonium, particulate chemical oxygen demand and temperature are also modelled using the same framework with high frequency data. The calibration is performed semi-automatically with two different methods depending on data availability. The ‘traditional’ variables are calibrated with the Bootstrap method while the pharmaceutical loads are estimated with a least squares approach. The simulation results demonstrate that the BSM2 influent generator can describe the dynamics of both traditional variables and pharmaceuticals. Lastly, the study is complemented with: 1) the generation of longer time series for IBU following the same catchment principles; 2) the study of the impact of in-sewer SMX biotransformation when estimating the average daily load; and, 3) a critical discussion of the results, and the future opportunities of the presented approach balancing model structure/calibration procedure complexity versus predictive capabilities.
Biphasic reaction systems are composed of immiscible aqueous and organic liquid phases where reactants, products, and catalysts are partitioned. These biphasic conditions point to novel synthesis paths, higher yields, and faster reactions, as well as facilitate product separation. The biphasic systems have a broad range of application, such as the manufacture of petroleum based chemicals, pharmaceuticals, and agro-bio products. Major considerations in the design and analysis of biphasic reaction systems are physical and chemical equilibria, kinetic mechanisms, and reaction rates.

The primary contribution of this thesis is the development of a systematic modelling framework for the biphasic reaction system. The developed framework consists of three modules describing phase equilibria, reactions and mass transfer, and material balances of such processes. Correlative and predictive thermodynamic models, including newly developed group-contribution electrolyte model (e-KT-UNIFAC), have been implemented to predict the partitioning and equilibria of electrolyte and non-electrolyte species for a wide variety of reacting substances. Reaction kinetics and mass transfer are described by non-elementary reaction rate laws. Extents of reaction are used to calculate the species material balances.

The resulting mathematical model contains temperature dependent reaction rate parameters, equilibrium constants, and partition coefficients; where only the reaction rates are to be regressed to a minimum of time-dependent data. The application of the framework is made to five distinct cases in order to highlight the performance of the model for correlating the data and predicting the overall rates, the ultimate amounts of product formation, the ultimate impurities amount, and the optimum operating condition using different organic solvents leading to an improved and innovative design of the system.

Geometry optimization of a fibrous scaffold based on mathematical modelling and CFD simulation of a dynamic cell culture

In tissue engineering, the development of a tissue essentially depends on supply of an adequate amount of nutrients and the design of a proper biophysical micro-environment for cells. The limitation of the available initial number of cells, expensive substances and time consuming experiments are the main bottlenecks in this type of processes. In this regard, mathematical modelling and computational fluid dynamics simulation (CFD) are powerful tools to identify an efficient and optimized design by providing reliable insights of the process. This study presents a mathematical model and CFD simulation of cartilage cell culture under a perfusion flow, which allows not only to characterize the supply of nutrients and metabolic products inside a fibrous scaffold, but also to assess the overall culture condition and predict the cell growth rate. Afterwards, the simulation results supported finding an optimized design of the scaffold within a new mathematical optimization algorithm that is proposed. The main concept of this optimization routine is to maintain a large effective surface while simultaneously keeping the shear stress level in an operating range that is expected to be supporting growth. Thereafter, it should be possible to gradually reach improved culture efficiency as defined in the objective function.
Global sensitivity analysis of computer-aided molecular design problem for the development of novel working fluids for power cycles

This study compares two methods for global sensitivity analysis as a new approach for the identification and ranking of target properties in molecular design problems: A modified Morris Screening technique and Monte Carlo based standard regression. The two methodologies are highlighted in a case study involving the design of a working fluid for an Organic Ranking Cycle (ORC) design for power generation. Morris Screening is found to be favorable over Monte Carlo based standard regression. Monte Carlo based standard regression cannot be applied, because the current model cannot be sufficiently linearized. For Morris Screening techniques the critical temperature, the critical pressure and the acentric factor of the working fluid has been identified as the target properties with the highest sensitivity to the net power output of the cycle.

Global information
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Glycerol as high-permittivity liquid filler in dielectric silicone elastomers

A recently reported novel class of elastomers was tested with respect to its dielectric properties. The new elastomer materials based on a commercially available poly(dimethylsiloxane) composition, which has been modified by embedding glycerol droplets into its matrix. The approach has two major advantages that make the material useful in a dielectric actuator. First, the glycerol droplets efficiently enhance the dielectric constant, which can reach astonishingly high values in the composite. Second, the liquid filler also acts as a softener that effectively decreases the elastic modulus of the composite. In combination with very low cost and easy preparation, the two property enhancements lead to an extremely attractive dielectric elastomer material. Experimental permittivity data are compared to various theoretical models that predict relative permittivity changes as a function of filler loading, and the applicability of the models is discussed. VC 2016 Wiley Periodicals, Inc. J. Appl. Polym. Sci. 2016, 133, 44153.

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BFI (2012): BFI-level 1
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.679 SNIP 0.909
Web of Science (2010): Indexed yes
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Web of Science (2009): Indexed yes
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Glycerol as high-permittivity liquid filler in dielectric silicone elastomers

A recently reported novel class of elastomers was tested with respect to its dielectric properties. The new elastomer material is based on a commercially available polydimethylsiloxane (PDMS) composition, which has been modified by embedding glycerol droplets into its matrix. The approach has two major advantages that make the material useful in a dielectric actuator. First, the glycerol droplets efficiently enhance the dielectric constant which can reach very high values in the composite. Second, the liquid filler also acts as a softener that effectively decreases the elastic modulus of the composite. In combination with very low cost and easy preparation, the two property enhancements lead to a very attractive dielectric elastomer material. Experimental permittivity data are compared to various theoretical models that predict relative-permittivity changes as a function of filler loading, and the applicability of the models is discussed.

General information
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Grain protein concentration and harvestable protein under future climate conditions. A study of 108 spring barley accessions

In the present study a set of 108 spring barley (H. vulgare L.) accessions were cultivated under predicted future levels of temperature and [CO2] as single factors and in combination (IPCC, AR5, RCP8.5). Across all genotypes, elevated [CO2] (700 ppm day/night) slightly decreased protein concentration by 5%, while elevated temperature (+5 °C day/night) substantially increased protein concentration by 29%. The combined treatment increased protein concentration across accessions by 8%. This was an increase less than predicted from strictly additive effects of the individual treatments.
Despite the increase in grain protein concentration, the decrease in grain yield at combined elevated temperature and elevated [CO2] resulted in 23% less harvestable protein. There was variation in the response of the 108 accessions, which might be exploited to at least maintain if not increase harvestable grain protein under future climate change conditions.

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- **Authors:** Ingvordsen, C. H. (Intern), Gislum, R. (Ekstern), Jørgensen, J. R. (Ekstern), Mikkelsen, T. N. (Intern), Stockmarr, A. (Intern), Bagger Jørgensen, R. (Intern)
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  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 2
  - Scopus rating (2014): SJR 2.781 SNIP 2.046 CiteScore 5.93
  - Web of Science (2014): Indexed yes
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  - Scopus rating (2013): SJR 2.626 SNIP 1.973 CiteScore 6
  - ISI indexed (2013): ISI indexed yes
  - BFI (2012): BFI-level 2
  - Scopus rating (2012): SJR 2.612 SNIP 1.936 CiteScore 5.47
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  - Scopus rating (2011): SJR 2.596 SNIP 1.865 CiteScore 5.19
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 2.336 SNIP 1.8
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  - Scopus rating (2009): SJR 2.344 SNIP 1.698
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 2
  - Scopus rating (2008): SJR 2.197 SNIP 1.528
  - Scopus rating (2007): SJR 2.274 SNIP 1.682
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 1.822 SNIP 1.384
  - Scopus rating (2005): SJR 1.715 SNIP 1.614
  - Web of Science (2005): Indexed yes
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Green silicone elastomer obtained from a counterintuitively stable mixture of glycerol and PDMS

A green and cheap silicone-based elastomer has been developed. Through the simple mixing-in of biodiesel-originating glycerol into commercially available polydimethylsiloxane (PDMS) pre-polymer, a glycerol-in-PDMS emulsion was produced. This counterintuitively stable mixture became a basis for obtaining elastomeric composites with uniformly distributed glycerol droplets. Various compositions, containing from 0 to 140 parts of glycerol per 100 parts of PDMS by weight, were prepared and investigated in terms of ATR-FTIR, broadband dielectric spectroscopy, mechanical properties as well as optical and scanning electron microscopy. The materials were proven additionally to exhibit a strong affinity to water, which was investigated by simple water absorption tests. Incorporating glycerol into PDMS decreased the Young's modulus of the composites yet the ultimate strain of the elastomer was not compromised, even in the presence of very high loadings. The conducted experiments highlight the great potential of this new type of elastomer and reveal some possible applications.
This study presents new group contribution (GC) models for the prediction of Lower and Upper Flammability Limits (LFL and UFL), Flash Point (FP) and Auto Ignition Temperature (AIT) of organic chemicals applying the Marrero/Gani (MG) method. Advanced methods for parameter estimation using robust regression and outlier treatment have been applied to achieve high accuracy. Furthermore, linear error propagation based on covariance matrix of estimated parameters was performed. Therefore, every estimated property value of the flammability-related properties is reported together with its corresponding 95%-confidence interval of the prediction. Compared to existing models the developed ones have a higher accuracy, are simple to apply and provide uncertainty information on the calculated prediction. The average relative error and correlation coefficient are 11.5% and 0.99 for LFL, 15.9% and 0.91 for UFL, 2.0% and 0.99 for FP as well as 6.4% and 0.76 for AIT. Moreover, the temperature-dependence of LFL property was studied. A compound specific proportionality constant ($K_{LFL}$) between LFL and temperature is introduced and an MG GC model to estimate $K_{LFL}$ is developed. Overall the ability to predict flammability-related properties including the corresponding uncertainty of the prediction can provide important information for a qualitative and quantitative safety-related risk assessment studies.
Group contribution modelling for the prediction of safety-related and environmental properties

We present a new set of property prediction models based on group contributions to predict major safety-related and environmental properties for organic compounds. The predicted list of properties includes lower and upper flammability limits, heat of combustion, auto ignition temperature, global warming potential and ozone depletion potential.

Process safety studies and environmental assessments rely on accurate property data. Safety data such as flammability limits, heat of combustion or auto ignition temperature play an important role in quantifying the risk of fire and explosions among others. Global warming potential and ozone depletion potential became a standard to analyze the environmental impact of processes and products.

In the early stage of process development and analysis, experimental values are often not available due to cost or time constraints. In this case property prediction models like group contribution (GC) models can estimate data. However, the estimation needs to be accurate, reliable and as little time-consuming as possible so that the models can be used on the fly.

In this study the Marrero and Gani group contribution (MR GC) method has been used to develop the models for safety-related and environmental properties. The method considers the group contribution in three levels: The contributions from a specific functional group (1st order parameters), from poly-functional (2nd order parameters) as well as from structural groups (3rd order parameters). The latter two classes of GC factors provide additional structural information beside the functional group. The contributions of all three factors are then summed up. For the database, DIPPR are used together with the reported measurement accuracy. For parameter estimation, a comprehensive statistical methodology was followed to improve prediction accuracy and reliability (95% confidence).

The method is simple and easy to apply. Taking into account higher order groups increases the accuracy. Furthermore, the application range is high due to the high number of considered functional and structural contributions.

A thorough uncertainty analysis provides information about the prediction error, which is important for communicating the reliability of the predicted values for the user for potential applications in process safety studies and environmental assessments.

Example application of the models are shown for a selected class of chemicals to highlight the application range of models.

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Highly Branched Bio-Based Unsaturated Polyesters by Enzymatic Polymerization
A one-pot, enzyme-catalyzed bulk polymerization method for direct production of highly branched polyesters has been developed as an alternative to currently used industrial procedures. Bio-based feed components in the form of glycerol, pentaerythritol, azelaic acid, and tall oil fatty acid (TOFA) were polymerized using an immobilized Candida antarctica lipase B (CALB) and the potential for an enzymatic synthesis of alkyds was investigated. The developed method enables the use of both glycerol and also pentaerythritol (for the first time) as the alcohol source and was found to be very robust. This allows simple variations in the molar mass and structure of the polyester without premature gelation, thus enabling easy tailoring of the branched polyester structure. The postpolymerization crosslinking of the polyesters illustrates their potential as binders in alkyds. The formed films had good UV stability, very high water contact angles of up to 141° and a glass transition temperature that could be controlled through the feed composition.

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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.157 SNIP 1.286 CiteScore 3.72
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.321 SNIP 1.619 CiteScore 3.85
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Scopus rating (2013): SJR 1.415 SNIP 1.666 CiteScore 4.07
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Scopus rating (2012): SJR 1.591 SNIP 1.8 CiteScore 3.74
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High-pressure oxidation of methane

Methane oxidation at high pressures and intermediate temperatures was investigated in a laminar flow reactor and in a rapid compression machine (RCM). The flow-reactor experiments were conducted at 700–900 K and 100 bar for fuel-air equivalence ratios (Φ) ranging from 0.06 to 19.7, all highly diluted in nitrogen. It was found that under the investigated conditions, the onset temperature for methane oxidation ranged from 723 K under reducing conditions to 750 K under stoichiometric and oxidizing conditions. The RCM experiments were carried out at pressures of 15–80 bar and temperatures of 800–1250 K under stoichiometric and fuel-lean (Φ=0.5) conditions. Ignition delays, in the range of 1–100 ms, decreased monotonically with increasing pressure and temperature. A chemical kinetic model for high-pressure methane oxidation was established, with particular emphasis on the peroxyde chemistry. The thermodynamic properties of CH₃OO and CH₃OOH, as well as the rate constants for the abstraction reactions CH₃OOH + CH₃ = CH₃OO + CH₄ and CH₃OH + CH₃ = CH₃O + CH₄, were calculated at a high level of theory. Model predictions were evaluated against the present data as well as shock tube data (1100–1700 K, 7–456 bar) and flame speeds (1–10 bar) from literature. The model yielded satisfactory predictions for the onset temperature as well as for most major species upon ignition in the flow reactor, but the concentration of particularly CH₃OH was severely underpredicted, indicating that further work is desirable.
on reactions of CH$_3$O and CH$_3$OO. Measured ignition delay times from the RCM tests were reproduced well by the model for high pressures, but underpredicted at 15 bar. For the shock tube and flame conditions, predictions were mostly within the experimental uncertainty. Prompt dissociation of HCO increased predicted flame speeds by up to 4 cm s$^{-1}$ but had little impact under flow reactor, RCM or shock tube calculations.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, DNV-GL Oil & Gas, University of Groningen, Argonne National Laboratory  
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Web of Science (2018): Indexed yes  
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Web of Science (2017): Indexed Yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 4.41 SJR 1.125 SNIP 2.165  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 2.919 SNIP 2.448 CiteScore 5.12  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 1.388 SNIP 2.347 CiteScore 3.78  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 2.925 SNIP 2.639 CiteScore 4.85  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): SJR 1.43 SNIP 2.88 CiteScore 4.12  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 3.318 SNIP 2.817 CiteScore 4.13  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 1.181 SNIP 2.548  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 2.984 SNIP 2.308  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 0.961 SNIP 2.326  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 3.165 SNIP 2.367  
Scopus rating (2006): SJR 2.019 SNIP 2.581  
Scopus rating (2005): SJR 2.363 SNIP 2.314  
Web of Science (2005): Indexed yes
High temperature and high pressure gas cell for quantitative spectroscopic measurements

A high temperature and high pressure gas cell (HTPGC) has been manufactured for quantitative spectroscopic measurements in the pressure range 1-200 bar and temperature range 300-1300 K. In the present work the cell was employed at up to 100 bar and 1000 K, and measured absorption coefficients of a CO$_2$-N$_2$ mixture at 100 bar and 1000 K are revealed for the first time, exceeding the high temperature and pressure combinations previously reported. This paper discusses the design considerations involved in the construction of the cell and presents validation measurements compared against simulated spectra, as well as published experimental data. (C) 2015 Elsevier Ltd. All rights reserved.
High Temperature Corrosion on Biodust Firing
The high content of alkali metals and chlorine in biomass gives rise to fouling/slagging and corrosion of heat exchange components, such as superheaters, in biomass fired power plants. Increasing the lifetime of these components, and in addition, preventing unwarranted plant shutdowns due to their failure, requires understanding of the complex corrosion mechanisms, as well as development of materials that are resistant to corrosion under biomass firing conditions, thereby motivating the current work.

To understand the mechanisms of corrosion attack, comprehensive analysis of corrosion products was necessary. In the present work, two complementary methodologies based on analysis of cross sections and plan views were applied to achieve comprehensive characterization of corrosion products. The suitability of these methods for both laboratory scale and full scale corrosion investigations was demonstrated by the combined use of complementary information from microscopy, energy dispersive X-ray spectroscopy and various X-ray diffraction characterization techniques.

In light of the wide variation in operating conditions in biomass fired power plants, systematic and well-controlled, but realistic laboratory scale exposures were carried out to understand the effect of process parameters such as gas phase chemistry, time and temperature variations, on the corrosion process. By conducting corrosion exposures under: oxidizing, oxidizing-chlorinating, oxidizing-sulphidizing and oxidizing-chlorinating-sulphidizing gas mixtures, it was possible to observe the contributions of chlorination, sulphation and sulphidation on the complex corrosion mechanisms. Comparative exposure of KCl-coated and KCl-free samples under each of the gas atmospheres revealed that the corrosion attack due to the presence of a deposit overrules the effect of the gas phase chemistry. Further, using the oxidizing-chlorinating-sulphidizing gas mixture corresponding to straw-firing conditions, the evolution of corrosion with time and temperature variation was studied. Corrosion attack does not decrease with time after longer exposures under isothermal conditions and is accelerated once the material encounters a higher temperature.

For the investigated austenitic stainless steels, FeCrAl alloys and Ni-based superalloy, the formation of a protective oxide layer that suppressed corrosion attack was not observed. However, it was established that among the alloying elements present in these alloys, Ni exhibits a relatively greater resistance to corrosion attack. Surface modification approaches with the aim to form resistant oxides or coatings on superheater surfaces were evaluated. This included preoxidation to obtain Al2O3 and Ti-Cr-rich oxides, as well as formation of SiOx coating, Ni electroplating and NiAl coatings on commercial alloys. For most of the modified surfaces, in particular α-Al2O3 obtained by preoxidation, poor mechanical integrity of the oxide layer nullifies its otherwise excellent chemical integrity towards corrosion attack. Nonetheless, corrosion attack on most of the modified surfaces was substantially lower than attack on the virgin alloys. Thus, with further optimization, these approaches may provide alternative corrosion resistant materials for application in biomass fired power plants.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Mechanical Engineering, Materials and Surface Engineering, CHEC Research Centre
Hybrid nanocellulose/nanoclay composites for food packaging applications

In this research, cellulose nanofibres (CNFs) were extracted and dispersed through a combination of alkali-acetylation treatments followed by soft mechanical treatments. Thereafter, PLA-based nanocomposites with CNF, nanocrystalline cellulose (CNC) and/or commercially available nanoclay (Cloisite™ 30B) were prepared and evaluated for use in food packaging. It was determined that composites with CNF or CNC and clay led to a great reduction in the oxygen transmission rate (OTR) and the water vapour transmission rate (WVTR) (up to a 90% reduction in the OTR and 76% in the WVTR for PLA/CNF 5%/C30B 5%). A significant increase in thermomechanical resistance was obtained (the storage modulus of PLA/CNF 5%/C30B 5% at 85°C, was 3.7 times higher than for neat PLA) and increased crystallisation kinetics (the PLA/CNF 1%/C30B 1% showed an 81% reduction in half-crystallisation time compared with neat PLA) without a significant reduction in optical properties at moderate nanoparticle loading.

Furthermore, it was found that solvent casting at a low temperature induced sub-micron-sized spherulites, which had little influence on water diffusion and transparency decline. On the other hand, high temperature processing led to larger spherulite sizes, which had a more significant impact on water diffusion and transparency reduction but also showed an increased water sorption. Finally, it was found that cellulose nanofibers reduced water diffusion to an extent similar to C30B (21% vs. 27%), while hybrid composites showed 49% decrease, albeit CNF based composites showed increased water sorption (7% for PLA/CNF 1% composite and 9% for PLA/CNF 1%/C30B 1% when compared with neat PLA). The reduced diffusivity of the hybrid nanocomposites suggested that the material was promising for active packaging, since low diffusivity leads to the slower release of active compounds such as essential oils. On top of that the CNF was surface modified with hydrocinnamic acid (gCNF), with the aim of reducing even more the release rate of carvacrol and to enhance the CNF dispersion with the PLA matrix. Consequently, carvacrol-loaded PLA/CNF, PLA/gCNF and hybrid PLA/CNF/C30B composites were prepared and evaluated on controlled release applications. It was established that the surface modification of CNF greatly enhanced the dispersion of the gCNF and that carvacrol loaded hybrid composites showed a decreased release rate, high ductility and a reduced WVTR which made those composites promising material for food packaging films.
Hybrid poly(lactic acid)/nanocellulose/nanoclay composites with synergistically enhanced barrier properties and improved thermomechanical resistance

Poly(lactic acid) (PLA)-based hybrid nanocomposites (PLA, nanoclay and nanocellulose) were prepared by reinforcing neat PLA with commercially available nanoclay (Cloisite C30B) and nanocellulose, in the form of either partially acetylated cellulose nanofibres (CNFs) or nanocrystalline cellulose. Composites with 1 or 5 wt% of nanocellulose, in combination with 1, 3 and 5 wt% of nanoclay, were prepared, and their barrier properties were investigated. It was found that the combination of clay and nanocellulose clearly resulted in synergistic behaviour in terms of the oxygen transmission rate (OTR) through a reduction of up to 90% in OTR and a further reduction in the water vapour transmission rate of up to 76%. In addition, the nanocomposite films showed improved thermomechanical resistance and improved crystallisation kinetics while maintaining high film transparency. This makes the hybrid PLA/CNF/C30B nanocomposites a very promising material for food packaging applications. © 2016 Society of Chemical Industry

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, University of British Columbia, Grenoble-INP Pagora
Authors: Trifol Guzman, J. (Intern), Plackett, D. (Ekstern), Sillard, C. (Ekstern), Szabo, P. (Intern), Bras, J. (Ekstern), Daugaard, A. E. (Intern)
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Journal: Polymer International
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.24 SJR 0.699 SNIP 0.778
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.743 SNIP 0.898 CiteScore 2.4
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.779 SNIP 0.953 CiteScore 2.31
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.818 SNIP 1.251 CiteScore 2.52
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.78 SNIP 1.039 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.809 SNIP 1.072 CiteScore 2.21
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.999 SNIP 0.969
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.107 SNIP 0.965
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.961 SNIP 1.008
Scopus rating (2007): SJR 0.89 SNIP 1.009
Scopus rating (2006): SJR 0.868 SNIP 1.058
Hydrate Equilibrium Data for CO2+N2 System in the Presence of Tetra-n-butylammonium Fluoride (TBAF) and Mixture of TBAF and Cyclopentane (CP)

Hydrates can be used for CO2 capture from flue gases (hydrate crystallization). In this work, hydrate equilibrium data were measured and compared with literature data. The isochoric method was used to determine the gas hydrate dissociation points. Different CO2+N2 gas mixtures were used in the presence of promoters such as tetra-n-butylammonium fluoride (TBAF) and mixtures of TBAF and cyclopentane (CP). The key novel aspect of this work is the use of a combination of promoters, TBAF and CP, which under certain conditions induced further pressure reduction in comparison to pure TBAF results. Concerning experiments with pure promoter, there is good agreement between our results and literature results for different gas mixtures and promoter concentrations.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Paris Tech
Authors: Tzirakis, F. (Intern), Stringari, P. (Ekstern), Coquelet, C. (Ekstern), von Solms, N. (Intern), Kontogeorgis, G. (Intern)
Pages: 1007-1011
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Main Research Area: Technical/natural sciences

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Journal: Journal of Chemical and Engineering Data
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Hydrate equilibrium data for the CO$_2$ + N$_2$ system with the use of tetra-n-butylammonium bromide (TBAB), cyclopentane (CP) and their mixture

Carbon Dioxide capture and sequestration (CCS) is nowadays an important area of research for decreasing CO$_2$ emissions worldwide. Hydrates can become of great importance in the future as they form the basis for a new technology that can be used for CO$_2$ capture from flue gases (hydrate crystallization). In this work hydrate equilibrium data are measured and compared with literature data. In particular, experimental results for hydrate dissociation with several promoters are presented. The isochoric method is used to determine the gas hydrate dissociation points. Different CO$_2$ + N$_2$ gas mixtures were used with presence of promoters such as tetra-n-butylammonium bromide (TBAB), cyclopentane (CP) and mixtures of TBAB with CP. The novelty of this work is the combination of promoters, TBAB and CP, which under certain conditions induced greater pressure reduction in comparison to pure TBAB results. Concerning experiments with pure promoters, there is excellent consistency between our results and literature results for different gas mixtures and promoter concentrations. Finally, experimental uncertainties for temperature, pressure, and molar composition are also presented.
Hydrodeoxygenation of phenol over Pd catalysts by in-situ generated hydrogen from aqueous reforming of formic acid

Hydrodeoxygenation of phenol, as model compound of bio-oil, was investigated over Pd catalysts, using formic acid as a hydrogen donor. The order of activity for deoxygenation of phenol with Pd catalysts was found to be: Pd/SiO₂ > Pd/MCM-41 > Pd/CA > Pd/Al₂O₃ > Pd/HY approximate to Pd/ZrO₂ ≈ Pd/CW > Pd/HSAPO-34 > Pd/HZSM-5. The good performance of Pd/SiO₂ is owing to its proper pore structure and large specific surface area. The high level of Bronsted acid sites in SiO₂ also favors the deoxygenation of phenol. (C) 2016 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Chinese Academy of Sciences
Authors: Zeng, Y. (Ekstern), Wang, Z. (Ekstern), Lin, W. (Ekstern), Song, W. (Ekstern), Christensen, J. M. (Intern), Jensen, A. D. (Intern)
Pages: 46-49
Publication date: 2016
Main Research Area: Technical/natural sciences
Hydrodeoxygenation of Phenol to Benzene and Cyclohexane on Rh(111) and Rh(211) Surfaces: Insights from Density Functional Theory

Herein we describe the C-O cleavage of phenol and cyclohexanol over Rh (111) and Rh (211) surfaces using density functional theory calculations. Our analysis is complemented by a microkinetic model of the reactions, which indicates that the C-O bond cleavage of cyclohexanol is easier than that of phenol and that Rh (211) is more active than Rh (111) for both reactions. This indicates that phenol will react mainly following a pathway of initial hydrogenation to cyclohexanol followed by hydrodeoxygenation to cyclohexane. We show that there is a general relationship between the transition state and the final state of both C-O cleavage reactions, and that this relationship is the same for Rh (111) and Rh (211).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, SLAC National Accelerator Laboratory
Authors: Garcia-Pintos, D. (Ekstern), Voss, J. (Ekstern), Jensen, A. D. (Intern), Studt, F. (Ekstern)
Pages: 18529-18537
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Main Research Area: Technical/natural sciences

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Journal: The Journal of Physical Chemistry Part C
Volume: 120
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Impact of different alginate lyases on combined cellulase–lyase saccharification of brown seaweed

Two bacterial polysaccharide lyase (PL) family 7 alginate lyases (EC 4.2.2.-) from Sphingomonas sp. (SALy) and Flavobacterium sp. (FALy), respectively, were selected for heterologous, monocomponent expression in Escherichia coli. The thermal stability, pH, and temperature reaction optima and substrate preferences of the enzymes on different alginate polymers were assessed and compared to those of a commercially available microbial alginate lyase (SigmALy). The optimal pH range for SALy was pH 5.5–7.0; for FALy and SigmALy it was pH 7.5. Reaction temperatures of 30–50 °C had no influence on the activity of any of the enzymes, but the thermal stability was reduced above 50 °C. The FALy enzyme preferred poly-mannuronic acid as substrate, but exhibited activity also on poly-guluronic acid, whereas the SALy had highest activity on poly-guluronic acid, and the SigmALy was active only on poly-guluronic acid. When applied together with a fungal cellulase preparation (Cellic®CTec2) at pH 6 and 40 °C on a glucan rich brown seaweed Laminaria digitata the viscosity decreased in the initial minutes while measurable alginate degradation occurred primarily within the first 1–2 hours of reaction. Whereas FALy and SALy addition catalyzed degradation of more alginate than SigmALy addition, only the SigmAly enabled release of 90% of the available glucose within 8 hours of combined enzyme treatment. The level of mannuronic acid moieties released was inversely proportional to the glucose release, indicating that the degradation of mannuronic acid blocks inhibited cellulase catalyzed glucose release from L. digitata. Nevertheless, combined alginate lyase and cellulase treatment for 24 hours released all potential glucose regardless of the applied lyase. The enzymatic treatment moreover induced solubilization of sulfated fucoidan, whereas most of the nitrogen was recovered in the residual seaweed solids.
Implementation of Near-Infrared Spectroscopy for In-Line Monitoring of a Dehydration Reaction in a Tubular Laminar Reactor

Production of active pharmaceutical ingredients (APIs), fine chemicals, food products, and so on has in recent years been focused on implementing process intensification and process optimization tools. Lower costs and higher selectivity as well as better sustainability and competitiveness are the main benefits. A good approach to achieve this is to perform continuous manufacturing together with satisfying process analytical technology (PAT) requirements. The example studied here is the dehydration reaction of 9-allyl-2-chlorothioxanthen-9-ol ("N714-allylcarbinol") to give a mixture of cis- and trans-9H-thioxanthene, 2-chloro-9-(2-propenylidene)-(9CI) ("N746-butadienes"). A simplified procedure for designing mesoscale tubular reactors is demonstrated together with performance outside of the normal operation windows (higher pressures and temperatures above normal boiling points of solvents). Noninvasive in-line real-time monitoring was established by using Fourier transform near-infrared (FT-NIR) spectroscopy and a suitable partial least squares (PLS) model. High prediction accuracy was achieved and additionally validated by using at-line FT-NIR spectroscopy and off-line HPLC analysis. The presence of impurities was noticed and partly identified in the form of polymers. It is important to note that substrates and products in this work are API intermediates in the production of zuclopenthixol, a product of H. Lundbeck A/S.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CHEC Research Centre, The Danish Polymer Centre, Technical University of Denmark, H. Lundbeck A/S
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Journal: Organic Process Research and Development
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.48 SJR 1.062 SNIP 0.859
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.318 SNIP 1.029 CiteScore 2.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 0.99 CiteScore 2.38
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.13 SNIP 0.977 CiteScore 2.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.185 SNIP 1.12 CiteScore 2.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.212 SNIP 0.914 CiteScore 2.22
Importance of the oxygen bond strength for catalytic activity in soot oxidation

The oxygen bond strength on a catalyst, as measured by the heat of oxygen chemisorption, is observed to be a very important parameter for the activity of the catalyst in soot oxidation. With both intimate contact between soot and catalyst (tight contact) and with the solids stirred loosely together (loose contact) the rate constants for a number of catalytic materials outline a volcano curve when plotted against their heats of oxygen chemisorption. However, the optima of the volcanoes correspond to different heats of chemisorption for the two contact situations. In both cases the activation energies for soot oxidation follow linear Brønsted-Evans-Polanyi relationships with the heat of oxygen chemisorption. Among the tested metal or metal oxide catalysts Co3O4 and CeO2 were nearest to the optimal bond strength in tight contact oxidation, while Cr2O3 was nearest to the optimum in loose contact oxidation. The optimum of the volcano curve in loose contact is estimated to occur between the bond strengths of α-Fe2O3 and α-Cr2O3. Guided by an interpolation principle FeaCrOx binary oxides were tested, and the activity of these oxides was observed to pass through an optimum for an FeCr2Ox binary oxide catalyst, which exhibited a rate constant at 550 °C that was 2.3 times higher than the one for pure α-Cr2O3 and 29 times higher than the one for pure α-Fe2O3.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Christensen, J. M. (Intern), Grunwaldt, J. (Intern), Jensen, A. D. (Intern)
Pages: 235-244
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Publication information

Journal: Applied Catalysis B: Environmental
Volume: 188
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Importance of the oxygen bond strength for catalytic activity in soot oxidation

**Brønsted-Evans-Polanyi relationshipa, Heat of chemisorption, Oxygen bond strength, Soot oxidation, Volcano curve**

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**Publication:** Research - peer-review › Journal article – Annual report year: 2016
Importance of Vanadium-Catalyzed Oxidation of SO2 to SO3 in Two-Stroke Marine Diesel Engines

Low-speed marine diesel engines are mostly operated on heavy fuel oils, which have a high content of sulfur and ash, including trace amounts of vanadium, nickel, and aluminum. In particular, vanadium oxides could catalyze in-cylinder oxidation of SO2 to SO3, promoting the formation of sulfuric acid and enhancing problems of corrosion. In the present work, the kinetics of the catalyzed oxidation was studied in a fixed-bed reactor at atmospheric pressure. Vanadium oxide nanoparticles were synthesized by spray flame pyrolysis, i.e., by a mechanism similar to the mechanism leading to the formation of the catalytic species within the engine. Experiments with different particle compositions (vanadium/sodium ratio) and temperatures (300–800 °C) show that both the temperature and sodium content have a major impact on the oxidation rate. Kinetic parameters for the catalyzed reaction are determined, and the proposed kinetic model fits well with the experimental data. The impact of the catalytic reaction is studied with a phenomenological zero-dimensional (0D) engine model, where fuel oxidation and SOx formation is modeled with a comprehensive gas-phase reaction mechanism. Results indicate that the oxidation of SO2 to SO3 in the cylinder is dominated by gas-phase reactions and that the vanadium-catalyzed reaction is at most a very minor pathway.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Mechanical Engineering, Thermal Energy, University of Zaragoza
Authors: Colom, J. M. (Ekstern), Alzueta, M. U. (Intern), Christensen, J. M. (Intern), Glarborg, P. (Intern), Cordtz, R. F. (Intern), Schramm, J. (Intern)
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.05
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
In-Flame Characterization of a 30 MWth Bio-Dust Flame

This work presents a comprehensive flame characterization campaign on an operating full-scale Danish power plant. Amagerværket Unit 1 (AMV1, 350 MWth, 12 identical burners on 3 burner levels) is 100% fuelled with wood dust burned in suspension and stabilized by swirling flows in a triple concentric low-NOx configuration. The measurements focus on a single 30 MWth flame and include: Quantification of the gas temperature, the gas phase composition: O2, CO, CO2, H2O, and light hydrocarbons by intrusive probe measurements. It also includes both seeded and unseeded 2D laser doppler anemometry (LDA) velocity measurements, flame shape observations by video imaging, and particle entrainment by high speed infrared (IR) imaging. The flame is characterized along the geometrical centreline as well as in the horizontal and vertical plane of the flame. The results shed light on the flame anatomy of a full-scale burner and provide a comprehensive data set that quantifies key parameters: Gas phase temperature, composition, and flow field required in order to evaluate the performance of CFD simulations of complex combustion systems.

Influence of nanocatalyst on oxidative coupling, steam and dry reforming of methane: A short review

The influence of nanocatalyst on three main reactions for natural gas conversion such as steam reforming, dry reforming and oxidative coupling of methane has been reviewed with an emphasis on the literatures' reports and results. Although literatures' experimental results showed that the conversion of methane over the nanocatalysts was higher than that obtained from the ordinary catalysts, there was no correlation between the conversion of methane and the average sizes of the nanoparticles. The results of some nanocatalyst are also compared to ordinary catalysts in the literature which shows the improved influence of nanoscale catalyst performance on methane conversion.
Influence of surface modified nano silica on alkyd binder before and after accelerated weathering

Introduction of nano fillers in exterior wood coatings is not straightforward. Influence on aging of polymer binder needs to be taken into account along with possible benefits that nano fillers can provide immediately after application. This study shows the influence of two differently modified hydrophobic nano silica on an alkyd binder for exterior wood coatings. One month after application, the highest strength and energy required to break the films was obtained with addition of 3% disilazane modified silica. Changes in tensile properties were accompanied with a small increase in glass transition temperature. However, the highest stability upon accelerated weathering, measured by ATR-IR and DMA, was for nano composites with the highest amount of nano filler. The reasons for the observed changes are discussed together with the appearance of a feature that is possibly a secondary relaxation of alkyd polymer.

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, University of Copenhagen, Dyrup A/S
Pages: 134-143
Publication date: 2016
Main Research Area: Technical/natural sciences
Influence of Torrefaction on Single Particle Combustion of Wood

This study focuses on the influence of torrefaction on the char reactivity, char yield, and combustion time of 3-5 mm spherical wood particles in a single particle combustion reactor (SPC) operating at a nominal temperature of 1231 °C. The devolatilization times were reduced and the char burnout times were increased with increasing torrefaction degree. The devolatilization time depended linearly on the particle mass. The torrefaction pretreatment resulted in a marked increase in char yield and char particle density but no intrinsic reactivity change as determined by thermogravimetric analysis. The char yield and char particle density increased from 9 wt % and 123 kg/m³ for raw particles to 14 wt % and 259 kg/m³ for particles pretreated at 290 °C for 4 h. The results of this study demonstrate that the higher char yield and density are the
main reasons for the longer combustion time of torrefied wood.

**General Information**
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, South China University of Technology
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.05
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes
Web of Science (2000): Indexed yes
Influence on nickel particle size on the hydrodeoxygenation of phenol over Ni/SiO₂

Hydrodeoxygenation (HDO) of phenol over nickel nano-particles of different size (5-22 nm) supported on SiO₂ has been investigated in a batch reactor at 275 °C and 100 bar. Deoxygenation was only observed as a consecutive step of initial hydrogenation of phenol at the given conditions. Both the hydrogenation and deoxygenation reaction were found to be Ni-particle size dependent. Rapid hydrogenation of phenol to cyclohexanol was achieved over the catalysts with large particles, while the rate of deoxygenation of cyclohexanol was slow. For the catalysts with small Ni particles, the opposite behavior was observed. Specifically, the turn over frequency (TOF) of hydrogenation was 85 times slower for 5 nm particles than for 22 nm particles. On the contrary, the TOF of cyclohexanol deoxygenation increased by a factor of 20 when decreasing the particle size from 20 nm to 5 nm. A simple kinetic model showed that the rate limiting step for phenol HDO shifted from deoxygenation to hydrogenation when the particle size was below 9-10 nm. Surface site population theory evidenced that the deoxygenation reactions were favored on step/corner sites, giving higher deoxygenation rates at small particles. For hydrogenation, the influence of particle size on the rate could be related to the size of the Ni facets with larger facets thus being better.
Inhibition and Promotion of Pyrolysis by Hydrogen Sulfide (H$_2$S) and Sulfanyl Radical (SH)
This study resolves the interaction of sulfanyl radical (SH) with aliphatic (C$_1$–C$_4$) hydrocarbons, using CBS-QB3 based calculations. We obtained the C–H dissociation enthalpies and located the weakest link in each hydrocarbon. Subsequent computations revealed that, H abstraction by SH from the weakest C–H sites in alkenes and alkynes, except for ethylene, appears noticeably exothermic. Furthermore, abstraction of H from propene, 1-buten e, and iso-buten e displays pronounced spontaneity (i.e., $\Delta_r G^\circ < -20$ kJ mol$^{-1}$ between 300–1200 K) due to the relatively weak allylic hydrogen bond. However, an alkyl radical readily abstracts H atom from H$_2$S, with H$_2$S acting as a potent scavenger for alkyl radicals in combustion processes. That is, these reactions proceed in the opposite direction than those involving SH and alkene or alkyn e species, exhibiting shallow barriers and strong spontaneity. Our findings demonstrate that the documented inhibition effect of hydrogen sulfide (H$_2$S) on pyrolysis of alkanes does not apply to alkenes and alkynes. During interaction with hydrocarbons, the inhibitive effect of H$_2$S and promoting interaction of SH radical depend on the reversibility of the H abstraction processes. For the three groups of hydrocarbon, Evans–Polanyi plots display linear correlations between the bond dissociation enthalpies of the abstracted hydrogens and the relevant activation energies. In the case of methane, we demonstrated that the reactivity of SH radicals toward abstracting H atoms exceeds that of HO$_2$ but falls below those of OH and NH$_2$ radicals.

General information
State: Published
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Inocula selection in microbial fuel cells based on anodic biofilm abundance of \textit{Geobacter sulfurreducens}

Microbial fuel cells (MFCs) rely on microbial conversion of organic substrates to electricity. The optimal performance depends on the establishment of a microbial community rich in electrogenic bacteria. Usually this microbial community is established from inoculation of the MFC anode chamber with naturally occurring mixed inocula. In this study, the electrochemical performance of MFCs and microbial community evolution were evaluated for three inocula including domestic wastewater (DW), lake sediment (LS) and biogas sludge (BS) with varying substrate loading ($L_{\text{sub}}$) and external resistance ($R_{\text{ext}}$) on the MFC. The electrogenic bacterium \textit{Geobacter sulfurreducens} was identified in all inocula and its abundance during MFC operation was positively linked to the MFC performance. The LS inoculated MFCs showed highest abundance (18\% ± 1\%) of \textit{G. sulfurreducens}, maximum current density ($I_{\text{max}} = (690 ± 30)\ mA\cdot m^{-2}$) and coulombic...
efficiency (CE = 29% ± 1%) with acetate as the substrate. Imax and CE increased to (1780 ± 30) mA·m⁻² and 58% ± 1%,
respectively, after decreasing the R_ext from 1000 Ω to 200 Ω, which also correlated to a higher abundance of *G.
sulfurreducens* (21% ± 0.7%) on the MFC anodic biofilm. The data obtained contribute to understanding the microbial
community response to L_sub and R_ext for optimizing electricity generation in MFCs.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Technical
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Scopus rating (2016): CiteScore 1.37 SJR 0.404 SNIP 0.741
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
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BFI (2014): BFI-level 1
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.517 SNIP 1.197 CiteScore 1.4
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Scopus rating (2011): SJR 0.514 SNIP 1.07 CiteScore 1.36
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 0.493 SNIP 0.747
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.414 SNIP 0.775
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Scopus rating (2008): SJR 0.265 SNIP 0.569
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.278 SNIP 0.528
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.305 SNIP 0.568
Scopus rating (2005): SJR 0.245 SNIP 0.605
Scopus rating (2004): SJR 0.225 SNIP 0.735
Scopus rating (2003): SJR 0.319 SNIP 0.424
Scopus rating (2002): SJR 0.187 SNIP 0.368
Scopus rating (2001): SJR 0.299 SNIP 0.545

This work proposes an integrated model-based framework for chemical product design and evaluation based on which the software, VPPD-Lab (The Virtual Product-Process Design Laboratory) has been developed. The framework allows the following options: (1) design a product using design templates, such as, single molecule products, formulated products, blended products, emulsified products and devices; (2) analyze the product by performing virtual experiments (product property and performance calculations); (3) create and add new product property and product performance models; (4) create new product design templates when the desired template is not available. The product design templates follow the same common steps in the workflow for a product type but have options to employ product specific property models, data and calculation routines, if necessary. This paper highlights the application of the templates for three case studies: (i) the design of a refrigeration cycle, (ii) a mixture/blend design problem involving lubricant design and (iii) a tailor-made product design of jet-fuels (blended chemical products).

Integrated Process Design and Control of Multi-element Reactive Distillation Processes

In this work, integrated process design and control of reactive distillation processes involving multi-elements is presented. The reactive distillation column is designed using methods and tools which are similar in concept to non-reactive distillation design methods, such as driving force approach. The methods employed in this work are based on equivalent element concept. This concept facilitates the representation of a multi-element reactive system as equivalent binary light and heavy key elements. First, the reactive distillation column is designed at the maximum driving force where through steady-state analysis it is shown that it has the least energy consumption and carbon footprint. Next, through analytical and dynamic analysis it is verified that the control structure, disturbance rejection and the controllability at the maximum driving force is the best compared to any other design alternative which does not operate at the maximum driving force.
Integrated Process Design, Control and Analysis of Intensified Chemical Processes

Process design and process control have been considered as independent problems for many years. In this context, a sequential approach is used where the process is designed first, followed by the control design. However, this sequential approach has its limitations related to dynamic constraint violations, for example, infeasible operating points, process overdesign or under-performance. Therefore, by using this approach, a robust performance is not always guaranteed. Furthermore, process design decisions can influence process control and operation. To overcome these limitations, an alternative approach is to tackle process design and controllability issues simultaneously, in the early stages of process design. This simultaneous synthesis approach provides optimal/near optimal operation and more efficient control of conventional (non-reactive binary distillation columns) as well as complex chemical processes; for example, intensified processes such as reactive distillation. Most importantly, it identifies and eliminates potentially promising design alternatives that may have controllability problems later. To date, a number of methodologies have been proposed and applied on various problems to address the interactions between process design and control, and they range from optimization-based approaches to model-based methods.

In this work, integrated process design and control of reactive distillation processes is considered through a computer-aided framework. To assure that design decisions give the optimum operational and economic performance, operability and controllability issues are considered simultaneously with the process design issues. Operability issues are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at imposed disturbances in the feed under normal operating conditions. First, a set design methods, similar in concept to design of non-reactive distillations, such as McCabe-Thiele and driving force approach are selected to design the reactive distillation column. Next, these design methods are extended using element concept to also include ternary as well as multicomponent reactive distillation processes. The element concept is used to translate a ternary system of compounds (A + B ↔ C) to a binary system of elements (WA and WB). When only two elements are needed to represent the reacting system of more than two compounds, a binary element system is identified. In the case of multi-element reactive distillation processes (where more than two elements are encountered) the equivalent element concept is used to translate a multicomponent (multi-element) system of compounds (A + B ↔ C + D) to a binary system of key elements (elements WHK and WK1). For an energy-efficient design, non-reactive driving force (for binary non-reactive distillation), reactive driving force (for binary element systems) and binary-equivalent driving force (for multicomponent reactive distillation) were employed. For both the McCabe-Thiele and driving force method, vapor-liquid equilibrium data are based on elements. It has been demonstrated that designing a reactive distillation column at the maximum driving force will result in the minimum energy consumption. Note, that the same principles that apply to a binary non-reactive compound system are valid also for a binary-element or a multi-element system. Therefore, it is advantageous to employ the element based method for multicomponent reaction-separation systems.

It is shown that the same design-control principles that apply to a non-reacting binary system of compounds are also valid for a reactive binary system of elements or multi-elements for distillation columns. Application of this framework shows that designing the reactive distillation process at the maximum driving force results in a feasible and reliable design of the process as well as the controller structure. Through analytical, steady-state and closed-loop dynamic analysis it is verified that the control structure, disturbance rejection and energy requirement of the reactive distillation column is better than any other operation point that is not at the maximum driving force. Furthermore, it is shown that the design at the maximum driving force can be both controlled using simple controllers such as PI as well as advanced controllers such as MPC.
Integration of chlorogenic acid recovery and bioethanol production from spent coffee grounds

Spent coffee grounds (SCG) are an abundant by-product of the coffee industry with a complex composition that makes them a promising feedstock for a biorefinery. The objective of this study was to evaluate SCG as a substrate for combined chlorogenic acid and bioethanol production after dilute acid hydrolysis. The effect of phenolics extraction on the downstream process was evaluated exhibiting no loss of sugars and an increase in the sugar release efficiency during the dilute acid hydrolysis. In order to suggest an economically feasible process, phenolics extraction and dilute acid hydrolysis prior to ethanol fermentation were optimised by means of experimental design. The responses of the designs were not only the efficiencies of the processes, but also a balance between product recovery and estimated costs. In both cases, decreased efficiencies obtained with low liquid-solid ratios were countervailed by increased products concentrations and higher economical performance. Under the optimised conditions, the purity of the phenolics extract (32%) could allow it to enter the market as a dietary supplement of chlorogenic acid, a product with high trade value. Moreover, a concentration of 3.9% (w/v) ethanol was reached upon fermentation of the hydrolysate of SCG after extraction and dilute acid hydrolysis.
**Intelligent Heat System – high energy efficient wood stoves with low emissions**

This development and demonstration project conducted by HWAM A/S and DTU Chemical Engineering has contributed to the development of an automatically controlled wood stove (HWAM IHS), which is on the market today. The new digital control system ensures optimal combustion conditions by keeping optimal temperatures and overall oxygen concentrations in the combustion chamber throughout a complete wood log combustion cycle.

This improved performance has been verified by field tests in private homes where measurements showed significant reduced emissions and higher efficiency for the IHS stoves compared to traditional manually controlled stoves. The tests also showed that in many cases it is impossible to visually tell if non-optimal combustion occurs. Also, in practice it is impossible to manually control the combustion air as fast and optimally as the automatically controlled air inlet valves. Emission measurements at the research wood stove set-up at DTU Chemical Engineering showed generally low emissions of particles, well below current standards, and high energy efficiency.

The highest emissions of CO, VOC and PM were seen in the ignition phase while only a small particle peak was observed in the flame phase. The CO emission in the char combustion phase increased due to decreasing temperature in freeboard – but almost no particle emissions were seen this combustion phase.

For the further optimization of the state of art technology of the IHS stoves developed in this project, the improvement of the tertiary air injection showed a considerable potential, which may result in an improved combustion and reduced pollutant emissions. Some important areas of future work include further development of control system sensors and measuring methods, and optimisation of the combustion process and chamber.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST)
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Number of pages: 34
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Interactive Matching between the Temperature Profile and Secondary Reactions of Oil Shale Pyrolysis

This article investigates the effect of the reactor temperature profile on the distribution and characteristics of the products from fixed-bed pyrolysis of oil shale. Experiments were performed in a one-stage fixed-bed reactor and in a two-stage fixed-bed reactor. In the one-stage reactor, the shale oil yield reached 7.40 wt % with a reactor temperature profile from 900 to 550 degrees C and decreased to 2.23 wt % with the reverse temperature profile. The effect of the temperature profile was investigated further in the two-stage fixed-bed reactor combining a pyrolysis stage operating at 550 degrees C and a shale char bed operating at different temperatures. At low temperatures (550 degrees C), severe cracking occurred, converting both heavy and light oil to carbon and gas. The desirably matched reactor temperature profile for high oil yield is discussed via analysis of the tendency of secondary reactions subject to the temperature of particles contacting primary volatiles.
Interference-Blind Microfluidic Sensor for Ascorbic Acid Determination by UV/vis Spectroscopy

A microfluidic sensor is developed and targeted at specific ingredients determination in drug/food/beverage matrices. The surface of a serpentine polydimethylsiloxane (PDMS) microchannel is modified by enzyme via physisorption. When solutions containing target ingredients pass through the microfluidic channel, enzyme-catalyzed reaction occurs and only converts the target molecules to its products. The whole process is monitored by an end-channel UV/vis spectroscopic detection. Ascorbate oxidase and L-ascorbic acid (AA) are taken as enzyme-substrate model in this study to investigate the feasibility of using the developed strategy for direct quantification of AA in standard solutions and complex matrices. A dietary supplement product, vitamin C tablet, is chosen as a model matrix to test the microfluidic bio-sensor in real-sample analysis. The results illustrate that the established microfluidic biosensor exhibits good reproducibility, stability, and anti-interference property. Technically, it is easy to realize, depends on low investment in chip fabrication, and simple instrumental procedure, where only UV/vis spectrophotometer is required. To sum up, the developed strategy is economical, specific, and accurate, and can be potentially used for fast quantification of ingredient in samples with complex matrix background. It is promising to be widely spread in food industry and quality control department.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, International Iberian Nanotechnology Laboratory, INESC Microsistemas e Nanotecnologias
Authors: Bi, H. (Ekstern), Oliveira Fernandes, A. C. (Intern), Cardoso, S. (Ekstern), Freitas, P. (Ekstern)
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BFI (2013): BFI-level 1
Interpenetrated polymer networks based on commercial silicone elastomers and ionic networks with high dielectric permittivity and self-healing properties

The dielectric elastomers (DEs) technology can be used in many advanced applications, such as actuators, generators and sensors, showing advantageous and promising properties[1]. However, the main disadvantage is the high driving voltage required for the actuation process which limits the applicability. One method used to avoid this limitation is to increase the dielectric permittivity of the material in order to improve the actuation response at a given field. Recently, interpenetrating polymer networks (IPNs) based on covalently cross-linked commercial silicone elastomers and ionic networks from amino- and carboxylic acid-functional silicones have been designed[2] (Figure 1). This novel system provides both the mechanical stability and the high breakdown strength given by the silicone part of the IPNs and the high permittivity and the softening effect of the ionic network. Thus these improved properties are achieved without consequently increased Young’s moduli and decreased breakdown strength compared, for example, with other silicone elastomers containing fillers. In particular, the interpenetrating systems show dielectric permittivity ε’ from 6.7 to 2 x 103 at low frequencies (0,1 Hz), and the commercial elastomers RT625 and LR3043/30 provide the best viscoelastic properties to the systems, since they maintain low viscous losses upon addition of ionic network. The values of the breakdown strength...
in all cases remain higher than that of the reference pure PDMS network (ranging from 45 V/μm to 90V/μm)[3]. In addition, the ionic part of the interpenetrating systems, based on non-covalent interactions, provides promising self-healing properties both upon mechanical rupture and upon electrical breakdown. The systems are capable of recovering and support more than 100% elongation of the reassembled samples (Figure 2). This additional advantage achieved by the IPNs represents an encouraging step forward in the challenge of increasing the life-time of the DEs.

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Ogliani, E. (Intern), Yu, L. (Intern), Skov, A. L. (Intern)
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Interpenetrated polymer networks based on commercial silicone elastomers and ionic networks with high dielectric permittivity and self-healing properties

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Introduction to Applied Colloid and Surface Chemistry
Colloid and Surface Chemistry is a subject of immense importance and implications both to our everyday life and numerous industrial sectors, ranging from coatings and materials to medicine and biotechnology.

How do detergents really clean? (Why can’t we just use water?) Why is milk ‘milky’? Why do we use eggs so often for making sauces? Can we deliver drugs in better and controlled ways? Coating industries wish to manufacture improved coatings e.g. for providing corrosion resistance, which are also environmentally friendly i.e. less based on organic solvents and if possible exclusively on water. Food companies want to develop healthy, tasty but also long-lasting food products which appeal to the environmental authorities and the consumer. Detergent and enzyme companies are working to develop improved formulations which clean more persistent stains, at lower temperatures and amounts, to the benefit of both the environment and our pocket. Cosmetics is also big business! Creams, lotions and other personal care products are really just complex emulsions.

All of the above can be explained by the principles and methods of colloid and surface chemistry. A course on this topic is
Investigation of the Gas Injection Effect on Asphaltene Onset Precipitation Using the Cubic-Plus-Association Equation of State

Miscible and immiscible gas flooding is one of the enhanced oil recovery (EOR) techniques that has been widely used to increase the oil production. One of the critical problems with gas flooding is that it generally aggravates the asphaltene precipitation, which further creates a flow assurance problem. Therefore, it is imperative to investigate beforehand the effect of gas injection into the reservoir from the modeling results. The cubic-plus-association (CPA) equation of state (EoS) has previously been applied to model the asphaltene onset precipitation condition. In this work, we adopt the modeling approach from the previous work and provide the conceptual base for it. Five different reservoir fluids are studied to validate whether the model is able to calculate the effect of different types (e.g., N2, CO2, and methane) and amounts (e.g., 10, 20, and 30 mol %) of gas injections in agreement with experimental data from the literature. We also investigate the model behavior to show the importance of the association term in the EoS for the selected modeling approach. Sensitivity of the model results when we calculate either two or three model parameters from the experimental data is also studied. Model dependency upon the saturates, aromatics, resins, and asphaltenes (SARA) analysis or molecular weight (MW) of asphaltene is also analyzed. In addition, a unique characteristic of the model for the given stock tank oil (STO) is identified, which does not change with different types and amounts of gas injections and also remains the same at upper and lower onset pressure boundaries. On the basis of this unique characteristic, a simple procedure to predict asphaltene phase envelope (APE) for the reservoir oil with relatively simple and few experimental data, performed on STO with n-pentane/n-heptane as a precipitant, is proposed. This proposed procedure avoids the need of high-pressure measurements of upper onset pressure (UOP).
Ionic Liquid Design and Process Simulation for Decarbonization of Shale Gas

Ionic liquids (ILs) have been receiving increasing attention as a potential decarbonization solvent. However, the enormous number of potential ILs that can be synthesized makes it challenging to search for the best IL for CO$_2$ removal from methane. In this work, a method was proposed to screen suitable ILs based on the COSMO-RS (conductor-like screening model for real solvents) model, an absorption mechanism, and experimental data. Besides the Henry’s constant, the viscosity and toxicity of ILs should also be taken into consideration for an industrial decarbonization process. Furthermore, process simulation was performed to evaluate the new IL-based decarbonization technology. Considering CO$_2$ solubility, CO$_2$/CH$_4$ selectivity and toxicity and viscosity of ILs, [bmim][NTf$_2$] has been screened to be the potential solvent among 90 classes of ILs. Based on reliable experimental data, a rigorous thermodynamic model was established. The simulation results have been found to agree well with the available experimental results. Two process flow sheet options, use of two single-stage flash operations or a multistage flash operation following the absorber, have been simulated and assessed. Compared with the well-known MDEA (methyl diethanolamine) process for CO$_2$ capture, the single-stage and multistage process alternatives would reduce the total energy consumption by 42.8% and 66.04%, respectively.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Chinese Academy of Sciences, Technical University of Denmark
Irreversible Change of the Pore Structure of ZIF-8 in Carbon Dioxide Capture with Water Coexistence

The performance of zeolitic imidazolate framework 8 (ZIF-8) for CO2 capture under three different conditions (wetted ZIF-8, ZIF-8/water slurry, and ZIF-8/water-glycol slurry) was systemically investigated. This investigation included the study of the pore structure stability of ZIF-8 by using X-ray diffraction, scanning electron microscopy, Fourier transform infrared spectroscopy, and Raman detection technologies. Our results show that the CO2 adsorption ability of ZIF-8 could be substantially increased under the existence of liquid water. However, the structure characterization of the recovered ZIF-8 showed an irreversible change of its framework, which occurs during the CO2 capture process. It was found that there is an irreversible chemical reaction among ZIF-8, water, and CO2, which creates both zinc carbonate (or zinc carbonate hydroxides) and single 2-methylimidazole crystals, and therefore the pore structure of ZIF-8 collapses. It is suggested therefore that care must be taken when using ZIF-8 or products containing ZIF-8 for gas capture, gas separation, or other applications where both water and acid gases coexist.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Southwest Petroleum University
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
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Sialidases (3.2.1.18) may exhibit trans-sialidase activity to catalyze sialylation of lactose if the active site topology is congruent with that of the Trypanosoma cruzi trans-sialidase (EC 2.4.1.-). The present work was undertaken to test the hypothesis that a particular aromatic sandwich structure of two amino acids proximal to the active site of the T. cruzi trans-sialidase infers trans-sialidase activity. On this basis, four enzymes with putative trans-sialidase activity were identified through an iterative alignment from 2909 native sialidases available in GenBank, which were cloned and expressed in Escherichia coli. Of these, one enzyme, SialH, derived from Haemophilus parasuis had an aromatic sandwich structure on the protein surface facing the end of the catalytic site (Phe168; Trp366), and was indeed found to exhibit trans-sialidase activity. SialH catalyzed production of the human milk oligosaccharide 3'-sialyllactose as well as the novel trans-sialylation product 3-sialyllactose using casein glycomacropeptide as sialyl donor and lactose as acceptor. The findings corroborated that Tyr119 and Trp312 in the T. cruzi trans-sialidase are part of an aromatic sandwich structure that confers trans-sialylation activity for lactose sialylation. The in silico identification of trans-glycosidase activity by rational active site topology alignment thus proved to be a quick tool for selecting putative trans-sialidases amongst a large group of glycosyl hydrolases. The approach moreover provided data that help understand structure-function relations of trans-sialidases.
K-capture by Al-Si based Additives in an Entrained Flow Reactor

A water slurry, consisting of KCl and Al-Si based additives (kaolin and coal fly ash) was fed into an entrained flow reactor (EFR) to study the K-capturing reaction of the additives at suspension-fired conditions. Solid products collected from the reactor were analysed with respect to total and water-soluble K content to quantify the extent of the K-capturing reaction. The results showed that under suspension-fired conditions (1100 °C-1450 °C), kaolin and coal fly ash can effectively capture gaseous KCl. When increasing the mass ratio of KCl to Al-Si additives in the reactants, the conversion of KCl to K-aluminosilicate decreased. When reaction temperature increased from 1100 °C to 1450 °C, the conversion of KCl does not change significantly, which differs from the trend observed in fixed-bed reactor.

Linear Viscoelastic and Dielectric Relaxation Response of Unentangled UPy-Based Supramolecular Networks

Supramolecular polymers possess versatile mechanical properties and a unique ability to respond to external stimuli. Understanding the rich dynamics of such associative polymers is essential for tailoring user-defined properties in many products. Linear copolymers of 2-methoxyethyl acrylate (MEA) and varying amounts of 2-ureido-4[1H]-pyrimidone (UPy) quadruple hydrogen-bonding side units were synthesized via free radical polymerization. Their linear viscoelastic response was studied via small amplitude oscillatory shear (SAOS). The measured linear viscoelastic envelope (LVE) resembles that of a well-entangled polymer melt with a distinct plateau modulus. Dielectric relaxation spectroscopy (DRS) was employed to independently examine the lifetime of hydrogen bond units. DRS reveals a high frequency α-relaxation associated with the dynamic glass transition, followed by a slower α*-relaxation attributed to the reversible UPy hydrogen bonds. This time scale is referred to as the bare lifetime of hydrogen bonding units. Using the sticky Rouse model and a renormalized lifetime, we predict satisfactorily the LVE response for varying amounts of UPy side groups. The deviation from the sticky Rouse prediction is attributed to polydispersity in the distribution of UPy groups along the chain backbone. We conclude that the response of associating polymers in linear viscoelasticity is general and does not depend on the chemistry of association, but rather on the polymer molecular weight (MW) and MW distribution, the number of stickers per chain, \( n_s \), and the distribution of stickers along the backbone.
Linking granulation performance with residence time and granulation liquid distributions in twin-screw granulation: An experimental investigation

Twin-screw granulation is a promising wet granulation technique for the continuous manufacturing of pharmaceutical solid dosage forms. A twin screw granulator displays a short residence time. Thus, the solid-liquid mixing must be achieved quickly by appropriate arrangement of transport and kneading elements in the granulator screw allowing the production of granules with a size distribution appropriate for tableting. The distribution of residence time and granulation liquid is governed by the field conditions (such as location and length of mixing zones) in the twin-screw granulator, thus contain interesting information on granulation time, mixing and resulting sub-processes such as wetting, aggregation and breakage. In this study, the impact of process (feed rate, screw speed and liquid-to-solid ratio) and equipment parameters (number of kneading discs and stagger angle) on the residence time (distribution), the granulation liquid-powder mixing and the resulting granule size distributions during twin-screw granulation were investigated. Residence time and axial mixing data was extracted from tracer maps and the solid-liquid mixing was quantified from moisture maps, obtained by monitoring the granules at the granulator outlet using near infra-red chemical imaging (NIR-CI). The granule size distribution was measured using the sieving method. An increasing screw speed dominantly reduced the mean residence time. Interaction of material throughput with the screw speed and with the number of kneading discs led to most variation in the studied responses including residence time and mixing capacity. At a high screw speed, granulation yield improved due to high axial mixing. However, increasing material throughput quickly lowers the yield due to insufficient mixing of liquid and powder. Moreover, increasing liquid-to-solid ratio resulted in more oversized granules, and the fraction of oversized granules further increased at higher throughput. Although an increasing number of kneading discs was found to be critical for achieving a uniform distribution of the granulation liquid, the granulation performance was hampered due to insufficient solid-liquid mixing capacity of the current kneading discs which is essential for wet granulation. Thus, a balance between material throughput and screw speed should be strived for in order to achieve a specific granulation time and solid-liquid mixing for high granulation yield. Additionally, more efforts are needed both in modification of the screw configuration as well as the geometry of the mixing elements to improve the mixing capacity of the twin-screw granulator. The results from the current experimental study improved the understanding regarding the interplay between granulation time and the axial and solid-liquid mixing responsible for the granulation performance in twin-screw wet granulation.

General information

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Publication information

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Web of Science (2017): Indexed Yes 
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Scopus rating (2016): SJR 1.223 SNIP 1.499 CiteScore 4.2
Web of Science (2016): Indexed yes 
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.156 SNIP 1.415 CiteScore 4.04
Web of Science (2015): Indexed yes 
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.994 SNIP 1.247 CiteScore 3.48
Web of Science (2014): Indexed yes 
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.038 SNIP 1.287 CiteScore 3.47
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Linking Hydrolysis Performance to *Trichoderma reesei* Cellulolytic Enzyme Profile

*Trichoderma reesei* expresses a large number of enzymes involved in lignocellulose hydrolysis and the mechanism of how these enzymes work together is too complex to study by traditional methods, e.g. by spiking with single enzymes and monitoring hydrolysis performance. In this study a multivariate approach, partial least squares regression, was used to see if it could help explain the correlation between enzyme profile and hydrolysis performance. Diverse enzyme mixtures were produced by *Trichoderma reesei* Rut-C30 by exploiting various fermentation conditions and used for hydrolysis of washed pretreated corn stover as a measure of enzyme performance. In addition, the enzyme mixtures were analyzed by liquid chromatography - tandem mass spectrometry to identify and quantify the different proteins. A multivariate model was applied for prediction of enzyme performance based on the combination of different proteins present in an enzyme mixture. The multivariate model was used for identification of candidate proteins that are correlated to enzyme performance on pretreated corn stover. A very large variation in hydrolysis performance was observed and this was clearly caused by the difference in fermentation conditions. Besides β-glucosidase, the multivariate model identified several xylanases, Cip1 and Cip2 as relevant proteins to study further.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.411 SNIP 1.163
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.613 SNIP 1.37 CiteScore 4.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.589 SNIP 1.401 CiteScore 4.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.621 SNIP 1.425 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.639 SNIP 1.366 CiteScore 4.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.668 SNIP 1.483 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.538 SNIP 1.357
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.491 SNIP 1.356
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.238 SNIP 1.288
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.368 SNIP 1.362
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.458 SNIP 1.43
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.123 SNIP 1.239
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.094 SNIP 1.249
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.041 SNIP 1.228
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.197 SNIP 1.278
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.07 SNIP 1.177
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.102 SNIP 1.541
Web of Science (2000): Indexed yes
Long-Term Stability of PEG-Based Antifouling Surfaces in a Marine Environment

The work presented here concerns the use of polyethylene glycol (PEG) to reduce marine biofouling on ship hulls. The long-term stability of PEG towards degradation in a marine environment is reviewed, and the results of experiments designed to test the degradation of polyethylene glycol moieties are disclosed. The results show how the degradation of different polyethers can be followed, both in laboratory accelerated conditions and real life exposure by size exclusion chromatography (SEC) and nuclear magnetic resonance spectroscopy (NMR). Preliminary results indicate the influence of the chemical structure and the end-group on the degradation of different PEG-containing compounds in accelerated conditions, while showing very little degradation in real exposure tests in seawater after 3 months. Further experiments will be discussed involving long-term stability and degradation pathways involved in the degradation of PEG.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Danish Polymer Centre
Authors: Noguer, A. C. (Intern), Kiil, S. (Intern), Hvilsted, S. (Intern)
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Main Research Area: Technical/natural sciences
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Long_Term_Stability_of_PEG_Based_Antifouling_Surfaces_in_a_Marine_Environment_COSI2015.pdf
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Long-term stability of PEG-based antifouling surfaces in seawater

Poly(ethylene glycol) (PEG) is a hydrophilic polymer that has been extensively used in the biomedical and marine environment due to its antifouling properties. In the biomedical field, PEG has been successfully used to functionalize surfaces due to its resistance to cell and nonspecific protein adsorption. However, the long-term stability of PEG has limited its use in some areas. In the shipping industry, there is a great need for long-term solutions to keep the hulls of the ships fouling-free. The long-term stability of PEG in polydimethylsiloxane (PDMS) fouling-release coatings is studied here, in both accelerated laboratory tests and real seawater conditions. This article shows how PEG-based copolymers, which have been exposed in fouling-release coatings to real-life seawater conditions, are isolated and compared to those exposed to accelerated laboratory testing with successful results. The influence of the chemistry of the PEG compounds, the chosen laboratory degrading agents, and the possible degradation pathways and products are discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Danish Polymer Centre, Hempel A/S
Authors: Noguer, A. C. (Intern), Olsen, S. M. (Ekstern), Hvilsted, S. (Intern), Kiil, S. (Intern)
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Low immediate scientific yield of the PhD among medical doctors

Background: We studied the scientific yield of the medical PhD program at all Danish Universities. Methods: We undertook a retrospective observational study. Three PhD schools in Denmark were included in order to evaluate the postdoctoral research production over more than 18 years through individual publications accessed by PubMed. Results: A total of 2686 PhD graduates (1995-2013) with a medical background were included according to registries from all PhD schools in Denmark. They had a median age of 35 years (interquartile range (IQR), 32-38) and 53 % were women at the time of graduation. Scientific activity over time was assessed independently of author-rank and inactivity was measured relative to the date of graduation. Factors associated with inactivity were identified using multivariable logistic regression. 88.6 % of the PhD theses were conducted in internal medicine vs. 11.4 % in surgery. During follow-up (median 6.9 years, IQR 3.0-11.7), PubMed data searches identified that 87 (3.4 %) of the PhD graduates had no publication after they graduated from the PhD program, 40 % had 5 or less, and 90 % had 30 or less. The median number of publications per year after PhD graduation was 1.12 (IQR 0.61-1.99) papers per year. About 2/3 of the graduates became inactive after 1 year and approximately 21 % of the graduates remained active during the whole follow-up. Female gender was associated with inactivity: adjusted odds ratio 1.59 (95 % confidence interval 1.24-2.05). Conclusions: The scientific production of Danish medic PhD graduates was mainly produced around the time of PhD-graduation. After obtaining the PhD-degree the scientific production declines suggesting that scientific advance fails and resources are not harnessed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Copenhagen
Matematisk beskrivelse af dielektrisk styrke

Dielektriske elastomerer (DE) er en relativ ny type materiale, som har stort potentiale blandt andet inden for medico- og energiteknologi.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Technical University of Denmark
Authors: Pham, M. (Ekstern), Riddersholm Petersen, F. (Ekstern), Silau, H. (Intern), Stabell, N. B. (Intern), Skov, A. L. (Intern)
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Measurement of oxygen transfer from air into organic solvents: Oxygen transfer from air into organic solvents

Background: The use of non-aqueous organic media is becoming increasingly important in many biotechnological applications in order to achieve process intensification. Such media can be used for example to directly extract poorly water-soluble toxic products from fermentations. Likewise many biological reactions require the supply of oxygen, most normally from air. However, reliable on-line measurements of oxygen concentration in organic solvents (and hence oxygen transfer rates from air to the solvent) has to date proven impossible due limitations in the current analytical methods.

Results For the first time, we demonstrate on-line oxygen measurements in non-aqueous media using a novel optical sensor. The sensor was used to measure oxygen concentration in various organic solvents including toluene, THF, isooctane, DMF, heptane and hexane (which have all been shown suitable for several biological applications). Subsequently, we measured the oxygen transfer rates from air into these organic solvents.

Conclusion The measurement of oxygen transfer rates from air into organic solvents using the dynamic method was established using the solvent resistant optical sensor. The feasibility of online oxygen measurements in organic solvents has also been demonstrated, paving the way for new opportunities in process control.

General information
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Organisations: CAPEC-PROCESS, Department of Chemical and Biochemical Engineering, Graz University of Technology
Authors: Ramesh, H. (Intern), Mayr, T. (Ekstern), Hobisch, M. (Ekstern), Borisov, S. (Ekstern), Klimant, I. (Ekstern), Krühne, U. (Intern), Woodley, J. M. (Intern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.94 SJR 0.843 SNIP 1.111
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.8 SNIP 0.967 CiteScore 2.55
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.942 SNIP 1.03 CiteScore 2.49
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.027 SNIP 1.196 CiteScore 2.82
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.136 SNIP 1.146 CiteScore 2.58
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.981 SNIP 0.963 CiteScore 2.28
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.887 SNIP 0.896
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.843 SNIP 0.941
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.805 SNIP 1.019
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.625 SNIP 0.856
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.676 SNIP 0.915
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.595 SNIP 0.921
Scopus rating (2004): SJR 0.648 SNIP 0.773
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.548 SNIP 1.082
Scopus rating (2002): SJR 0.698 SNIP 1.073
Scopus rating (2001): SJR 0.648 SNIP 0.989
Scopus rating (2000): SJR 0.627 SNIP 1.046
Scopus rating (1999): SJR 0.645 SNIP 1.089

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Measurement of properties and pilot testing. CERE lab and model development

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Authors: Fosbøl, P. L. (Intern)
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Mechanical and Electrical Ageing Effects on the Long-Term Stretching of Silicone Dielectric Elastomers with Soft Fillers: Long-Term Stretching of Silicone Dielectric Elastomers
Dielectric elastomer materials for actuators need to be soft and stretchable while possessing high dielectric permittivity. Soft silicone elastomers can be obtained through the use of silicone oils, while enhanced permittivity can be obtained through the use of dipolar groups on the polymer backbone. Such elastomers are prepared by adding soft fillers to a strong and relatively stiff elastomer, Elastosil LR3043/50. The long-term stability of the materials is tested by straining the elastomers 60% statically for up to 3 months. The results show that soft fillers significantly influence the long-term stability of silicone elastomers, with electrical breakdown strength being the most influenced. Especially high concentrations of silicone oils should be avoided for long-term mechanical stability.

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Madsen, F. B. (Intern), Zakaria, S. B. (Intern), Yu, L. (Intern), Skov, A. L. (Intern)
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Scopus rating (2016): CiteScore 2.07 SJR 0.826 SNIP 1.083
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.807 SNIP 1.045 CiteScore 1.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.805 SNIP 1.089 CiteScore 1.66
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.733 SNIP 0.843 CiteScore 1.59
Mechanically compliant electrodes and dielectric elastomers from PEG-PDMS copolymers

Soft conducting elastomers have been prepared from polydimethylsiloxane-polyethylene glycol (PDMS-PEG) copolymer and surfactant-stabilized multi-walled carbon nanotubes (MWCNTs). The copolymer was chain-extended with PDMS of molecular weight 17.2 kg mol$^{-1}$ in order to obtain a crosslinkable PDMS with molecular weight around 20 – 30 kg mol$^{-1}$. MWCNTs were treated with surfactant and sonicated for better dispersion in the polymer matrix. The conductivity and mechanical properties of conducting elastomers were thoroughly investigated including stress and strain at break. The developed conducting elastomers showed high conductivity combined with inherent softness. The high conductivity and softness, PDMS-PEG copolymers with incorporated MWCNTs hold great promises as compliant and highly stretchable electrodes for stretchable devices such as electro-mechanical transducers.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: A Razak, A. H. (Intern), Madsen, F. B. (Intern), Skov, A. L. (Intern)
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Publication date: 2016
Main Research Area: Technical/natural sciences
Mechanics of the Separating Surface for a Two-Phase Co-current Flow in a Porous Medium

A mechanical description of an unsteady two-phase co-current flow in a porous medium is developed based on the analysis of the geometry and motion of the surface separating the two phases. It is demonstrated that the flow should be considered as essentially three-dimensional, even if the phase velocities are co-directed, since the phase interface is on average inclined to the direction of the flow. Kinematics of the flow is described, distinguishing between the average velocities of the bulk phases and their velocity near the interface between them. Dynamics of the flow is analyzed by means of the extended Maxwell-Stefan formalism, as in our previous paper (Shapiro 2015). Force balances are formulated in the directions parallel and orthogonal to the flow. A complete system of the flow equations, generalizing the traditional Buckley–Leverett and Rappoport–Leas system, is derived. Sample computations show that one of the main effects produced by the new system is sharpening of the displacement front, which otherwise would be washed out by the capillary forces, as in the solution of the Rappoport–Leas equation.
Mechanistic Models for Process Development and Optimization of Fed-batch Fermentation Systems

This work discusses the application of mechanistic models to pilot scale filamentous fungal fermentation systems operated at Novozymes A/S. For on-line applications, a state estimator model is developed based on a stoichiometric balance in order to predict the biomass and product concentration. This is based on on-line gas measurements and ammonia addition flow rate measurements. Additionally, a mechanistic model is applied offline as a tool for batch planning, based on definition of the process back pressure, aeration rate and stirrer speed. This allows the batch starting fill to be planned, taking into account the oxygen transfer conditions, as well as the evaporation rates of the system. Mechanistic models are valuable tools which are applicable for both process development and optimization. The state estimator described will be a valuable tool for future work as part of control strategy development for on-line process control and optimization.

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This work discusses the application of mechanistic models to pilot scale filamentous fungal fermentation systems operated at Novozymes A/S. For on-line applications, a state estimator model is developed based on a stoichiometric balance in order to predict the biomass and product concentration. This is based on on-line gas measurements and ammonia addition flow rate measurements. Additionally, a mechanistic model is applied offline as a tool for batch planning, based on definition of the process back pressure, aeration rate and stirrer speed. This allows the batch starting fill to be planned, taking into account the oxygen transfer conditions, as well as the evaporation rates of the system. Mechanistic models are valuable tools which are applicable for both process development and optimization. The state estimator described will be a valuable tool for future work as part of control strategy development for on-line process control and optimization.
Methane production enhancement by an independent cathode in integrated anaerobic reactor with microbial electrolysis

Anaerobic digestion (AD) represents a potential way to achieve energy recovery from waste organics. In this study, a novel bioelectrochemically-assisted anaerobic reactor is assembled by two AD systems separated by anion exchange membrane, with the cathode placing in the inside cylinder (cathodic AD) and the anode on the outside cylinder (anodic AD). In cathodic AD, average methane production rate goes up to 0.070 mL CH4/mL reactor/day, which is 2.59 times higher than AD control reactor (0.027 m3 CH4/m3/d). And COD removal is increased ~15% over AD control. When changing to sludge fermentation liquid, methane production rate has been further increased to 0.247 mL CH4/mL reactor/day (increased by 51.53% comparing with AD control). Energy recovery efficiency presents profitable gains, and economic revenue from increased methane totally self-cover the cost of input electricity. The study indicates that cathodic AD could cost-effectively enhance methane production rate and degradation of glucose and fermentative liquid.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Harbin Institute of Technology, Chinese Academy of Sciences
Authors: Cai, W. (Ekstern), Han, T. (Ekstern), Guo, Z. (Ekstern), Varrone, C. (Intern), Wang, A. (Ekstern), Liu, W. (Ekstern)
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Scopus rating (2014): SJR 2.41 SNIP 2.104 CiteScore 5.3
Web of Science (2014): Indexed yes
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Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 2.314 SNIP 2.508 CiteScore 5.56
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Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
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Microbial decomposition of keratin in nature—a new hypothesis of industrial relevance

Discovery of keratin-degrading enzymes from fungi and bacteria has primarily focused on finding one protease with efficient keratinase activity. Recently, an investigation was conducted of all keratinases secreted from a fungus known to grow on keratinaceous materials, such as feather, horn, and hooves. The study demonstrated that a minimum of three keratinases is needed to break down keratin, an endo-acting, an exo-acting, and an oligopeptide-acting keratinase.

Further, several studies have documented that disruption of sulfur bridges of the keratin structure acts synergistically with the keratinases to loosen the molecular structure, thus giving the enzymes access to their substrate, the protein structure. With such complexity, it is relevant to compare microbial keratin decomposition with the microbial decomposition of well-studied polymers such as cellulose and chitin. Interestingly, it was recently shown that the specialized enzymes, lytic polysaccharide monoxygenases (LPMOs), shown to be important for breaking the recalcitrance of cellulose and chitin, are also found in keratin-degrading fungi. A holistic view of the complex molecular self-assembling structure of keratin and knowledge about enzymatic and boosting factors needed for keratin breakdown have been used to formulate a hypothesis for mode of action of the LPMOs in keratin decomposition and for a model for degradation of keratin in nature. Testing such hypotheses and models still needs to be done. Even now, the hypothesis can serve as an inspiration for designing industrial processes for keratin decomposition for conversion of unexploited waste streams, chicken feather, and pig bristles into bioaccessible animal feed.
Microbial electrolysis contribution to anaerobic digestion of waste activated sludge, leading to accelerated methane production

Methane production rate (MPR) in waste activated sludge (WAS) digestion processes is typically limited by the initial steps of complex organic matter degradation, leading to a limited MPR due to sludge fermentation speed of solid particles. In this study, a novel microbial electrolysis AD reactor (ME-AD) was used to accelerate methane production for energy recovery from WAS. Carbon bioconversion was accelerated by ME producing H2 at the cathode. MPR was enhanced to 91.8 gCH4/m3 reactor/d in the microbial electrolysis ME-AD reactor, thus improving the rate by 3 times compared to control conditions (30.6 gCH4/m3 reactor/d in AD). The methane production yield reached 116.2 mg/g VSS in the ME-AD reactor. According to balance calculation on electron transfer and methane yield, the increased methane production was mostly dependent on electron contribution through the ME system. Thus, the use of the novel ME-AD reactor allowed to significantly enhance carbon degradation and methaneproduction from WAS.
Background: Bioelectrochemical systems have been considered a promising novel technology that shows an enhanced energy recovery, as well as generation of value-added products. A number of recent studies suggested that an enhancement of carbon conversion and biogas production can be achieved in an integrated system of microbial electrolysis cell (MEC) and anaerobic digestion (AD) for waste activated sludge (WAS). Microbial communities in integrated system would build a thorough energetic and metabolic interaction network regarding fermentation communities and electrode respiring communities. The characterization of integrated community structure and community shifts is not well understood, however, it starts to attract interest of scientists and engineers. Results: In the present work, energy recovery and WAS conversion are comprehensively affected by typical pretreated biosolid characteristics. We investigated the interaction of fermentation communities and electrode respiring communities in an integrated system of WAS fermentation and MEC for hydrogen recovery. A high energy recovery was achieved in the MECs feeding WAS fermentation liquid through alkaline pretreatment. Some anaerobes belonging to Firmicutes (Acetoanaerobium, Acetobacterium, and Fusibacter) showed synergistic relationship with exoelectrogens in the degradation of complex organic matter or recycling of MEC products (H2). High protein and polysaccharide but low fatty acid content led to the dominance of Proteiniciasticum and Parabacteroides, which showed a delayed contribution to the extracellular electron transport leading to a slow cascade utilization of WAS. Conclusions: Efficient pretreatment could supply more short-chain fatty acids and higher conductivities in the fermentative liquid, which facilitated mass transfer in anodic biofilm. The overall performance of WAS cascade utilization was substantially related to the microbial community structures, which in turn...
depended on the initial pretreatment to enhance WAS fermentation. It is worth noting that species in AD and MEC communities are able to build complex networks of interaction, which have not been sufficiently studied so far. It is therefore important to understand how choosing operational parameters can influence reactor performances. The current study highlights the interaction offermentative bacteria and exoelectrogens in the integrated system.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Chinese Academy of Sciences, Harbin Institute of Technology, Taiyuan University of Technology
Authors: Liu, W. (Ekstern), He, Z. (Ekstern), Yang, C. (Ekstern), Zhou, A. (Ekstern), Guo, Z. (Ekstern), Liang, B. (Ekstern), Varrone, C. (Intern), Wang, A. (Ekstern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.414 SNIP 1.722 CiteScore 5.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.17 SNIP 1.815 CiteScore 6.21
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Scopus rating (2012): SJR 2.15 SNIP 1.849 CiteScore 5.7
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**Bibliographical note**
Microfluidic device for continuous single cells analysis via Raman spectroscopy enhanced by integrated plasmonic nanodimers

In this work a Raman flow cytometer is presented. It consists of a microfluidic device that takes advantage of the basic principles of Raman spectroscopy and flow cytometry. The microfluidic device integrates calibrated microfluidic channels—where the cells can flow one-by-one—, allowing single cell Raman analysis. The microfluidic channel integrates plasmonic nanodimers in a fluidic trapping region. In this way it is possible to perform Enhanced Raman Spectroscopy on single cell. These allow a label-free analysis, providing information about the biochemical content of membrane and cytoplasm of each cell. Experiments are performed on red blood cells (RBCs), peripheral blood lymphocytes (PBLs) and myelogenous leukemia tumor cells (K562).

General information

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Università “Magna Graecia” of Catanzaro, King Abdullah University of Science and Technology, Politecnico di Milano
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Scopus rating (2015): SJR 1.976 SNIP 1.755 CiteScore 3.78
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 2.349 SNIP 2.166 CiteScore 4.18
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.358 SNIP 2.226 CiteScore 4.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.587 SNIP 2.145 CiteScore 3.85
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.579 SNIP 2.606 CiteScore 4.04
Miscanthus as energy crop: Environmental assessment of a miscanthus biomass production case study in France

The cultivation of miscanthus (Miscanthus x Giganteus) as biomass for energy production has increased year by year due to its agronomical performances. In particular, in France, miscanthus is cultivated in the Bourgogne region and it is used as feedstock to produce pellet. In this paper, emergy assessment of different logistic (harvesting) strategies for miscanthus production in the Bourgogne region is presented. Emergy assessment is a particular methodology suited to quantify the resource use of a process and to estimate the percentage of renewability of products or services. The case study includes all phases to grow miscanthus, harvest the biomass as chips or short- or long-stranded bales and distribute it to a bioenergy plant. The aim of this study is to evaluate the sustainability performance of the whole process, from the field to the plant's gate. The emergy flow that represents the environmental cost of the whole process, the percentage of renewability (%R) and the Unit Emergy Values (UEV) that represent the resource use efficiency of the final products for each phase are calculated. Since miscanthus is reproduced by rhizomes, in addition to the system for growing and distributing miscanthus biomass, the system for producing miscanthus rhizomes is also analysed and a UEV for miscanthus rhizomes of 1.19E+05 seJ/J was obtained. Moreover, due the absence of other emergy assessments for miscanthus biomass for comparison, a sensitivity analysis has been made by considering different transport distances and different aboveground biomass yields. Comparing the harvesting methodologies, the bales made with short strands has the best performance. The aboveground biomass production was found to have an Energy Return On energy Investment (EROI), which is the double of that from an experimental miscanthus field in Italy. However, this implied a trade-off for the net energy production of about 50%.
General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, AgroParisTech
Authors: Morandi, F. (Intern), Perrin, A. (Ekstern), Østergård, H. (Intern)
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Scopus rating (2016): CiteScore 5.83 SJR 1.615 SNIP 2.382
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.609 SNIP 2.383 CiteScore 5.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.661 SNIP 2.477 CiteScore 4.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.644 SNIP 2.581 CiteScore 4.47
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.706 SNIP 2.328 CiteScore 4.07
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.461 SNIP 1.825 CiteScore 3.19
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
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Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 0.942 SNIP 1.544
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.813 SNIP 1.354
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.942 SNIP 1.489
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.842 SNIP 1.543
Scopus rating (2005): SJR 0.544 SNIP 1.357
Scopus rating (2004): SJR 0.753 SNIP 1.818
Scopus rating (2003): SJR 0.501 SNIP 1.152
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.481 SNIP 1.103
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.419 SNIP 0.85
Model-based analysis of a twin-screw wet granulation system for continuous solid dosage manufacturing

Implementation of twin-screw granulation in a continuous from-powder-to-tablet manufacturing line requires process knowledge development. This is often pursued by application of mechanistic models incorporating the underlying mechanisms. In this study, granulation mechanisms considered to be dominant in the kneading element regions of the granulator i.e., aggregation and breakage, were included in a one-dimensional population balance model. The model was calibrated using the experimentally determined inflow granule size distribution, and the mean residence time was used as additional input to predict the outflow granule size distribution. After wetting, the first kneading block caused an increase in the aggregation rate which was reduced afterwards. The opposite was observed in case of the breakage rate. The successive kneading blocks lead to a granulation regime separation inside the granulator under certain process conditions. Such a physical separation between the granulation regimes is promising for future design and advanced control of the continuous granulation process. (C) 2016 Elsevier Ltd. All rights reserved.
Model-Based Monitoring of an Industrial Batch Pectin Extraction

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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, CP Kelco ApS
Authors: André Fernandes Caroço, R. (Intern), Santacoloma, P. A. (Ekstern), Abildskov, J. (Ekstern), Huusom, J. K. (Intern)
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Modeling and Evaluation of Bioenergy and Agriculture System Integration
This Ph.D thesis focuses on exploring the integration between agriculture and bioenergy, by developing and analysing biomass fuelled energy system concepts that can produce heat and power in the effort of replacing fossil fuelled
production. Bioenergy technologies based on thermochemical and biochemical conversion have been developed to utilize residual resources from agricultural systems. Nevertheless, these technologies are more often used in systems that maximize energy generation while disregarding and destroying the "waste" products which often contain essential elements to agriculture. Those type of systems could then eventually lead to soil depletion and contribute to mineral resource scarcity. New energy system concepts are developed in this thesis that 1) maximize biomass utilization for heat and power generation 2) while maintaining soil quality and 3) decrease consumption of mineral fertilizers in the agricultural system.

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Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Sigurjonsson, H. Æ. (Intern), Elmegaard, B. (Intern), Ahrenfeldt, J. (Intern), Clausen, L. R. (Intern)
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Modeling a production scale milk drying process: parameter estimation, uncertainty and sensitivity analysis
A steady state model for a production scale milk drying process was built to help process understanding and optimization studies. It involves a spray chamber and also internal/external fluid beds. The model was subjected to a comprehensive statistical analysis for quality assurance using sensitivity analysis of inputs/parameters, and uncertainty analysis to estimate confidence intervals on parameters and model predictions (error propagation). Variance based sensitivity analysis (Sobol's method) was used to quantify the influence of inputs on the final powder moisture as the model output. Bayesian Inference using Markov Chain Monte Carlo sampling was used to quantify the uncertainty on the estimated parameters using available process data. In a full scale process the inputs with major range of variation are: moisture content at concentrate chamber feed (variation around 4%), and humidity at chamber inlet air (variation > 100%). The sensitivity analysis results suggest exploring improvements in the current control (Proportional Integral Derivative) for moisture content at concentrate chamber feed in order to reduce the output variance. It is also confirmed that humidity control at chamber inlet air stream would not be necessary because, despite its wide range of variation (air taken from outside), its impact on output variance is low. The uncertainty analysis results showed that confidence intervals obtained for parameters were reasonable, although some of them were found significantly correlated. For model applications, this means that model simulations should be performed using not only parameter values but also their correlation matrix by means of non-linear error propagation methods such as Monte Carlo techniques. The separate effects on model prediction uncertainties due to parameter estimation and measurement errors were studied. The results indicate that the error in measurements is the main responsible for the uncertainty in output predictions. Therefore using proper filtering of measurements, the comprehensively tested model is ready to support simulation based efforts for further process optimization. (C) 2016 Elsevier Ltd. All rights reserved.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad de la Republica
Authors: Ferrari, A. (Ekstern), Gutierrez, S. (Ekstern), Sin, G. (Intern)
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Modeling derivative properties and binary mixtures with \( \text{CO}_2 \) using the CPA and the quadrupolar CPA equations of state

The cubic plus association (CPA) equation of state (EoS) is extended to include quadrupolar interactions. The quadrupolar term is based on a modification of the perturbation terms by Larsen et al. (1977) [5] for a hard sphere fluid with a symmetric point quadrupole moment. The new quadrupolar CPA (qCPA) can be used without introducing any additional pure compound parameters. Alternatively a single additional adjustable parameter can be employed. To evaluate qCPA several pure compound properties are predicted. The model is furthermore evaluated for its ability to predict and correlate binary vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE) of mixtures containing \( \text{CO}_2 \) and hydrocarbons, water, alcohols, or selected quadrupolar compounds. The results indicate that most pure compound property predictions are satisfactory but similar to other CPA approaches. When binary mixtures are considered, qCPA appear to offer a systematic improvement as compared to the cases where quadrupolar interactions are ignored. This improvement is particularly pronounced when mixtures of \( \text{CO}_2 \) and hydrocarbons are considered, where the model is almost fully predictive. Using the same modeling approach qCPA can accurately correlate both the phase behaviour of \( \text{CO}_2 \) +hydrocarbon mixtures as well as mixtures of \( \text{CO}_2 \)+a self-associating compound.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Bjørner, M. G. (Intern), Kontogeorgis, G. (Intern)
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Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
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Modeling of Asphaltene Onset Precipitation Conditions with Cubic Plus Association (CPA) and Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) Equations of State

Asphaltene precipitation has been one of the major problems in the oil industry, and its modeling is still believed to be a quite complex issue due to the different characteristics of thousands of heavy components in crude oil. There have been several attempts to model asphaltene precipitation using various equations of state and empirical models. In the past few years, association models based on CPA and SAFT equations of state have been found to be promising models for studies of asphaltene precipitation. In this work, we compare asphaltene precipitation results obtained from different modeling approaches based on CPA, PC-SAFT with association (PC-SAFT (WA)), and PC-SAFT without association (PC-SAFT (WOA)) models. While the modeling approaches for the CPA and PC-SAFT (WOA) have been described before in various literature, the modeling approach for PC-SAFT (WA) is proposed in this work: All three models require the same number of experimental data points (at least three upper onset pressures and one bubble pressure) in order to obtain model parameters. Different types of asphaltene phase behavior for different reservoir fluids, where asphaltene solubility either decreases or increases with temperature, and where asphaltene precipitation occurs during reservoir fluid depressurization, and the effect of gas injection are studied in order to investigate thoroughly the potential and reliability of the models. A total of five reservoir fluids and one model oil are studied with all three models. It is found that the modeling
approach with the CPA EoS is more reliable compared to the other two approaches used in this study. The advantage of the association term to describe interactions between asphaltene and other stock tank oil (STO) heavy components is also evident from this study. The sensitivity of SARA data to the modeling approach based on PC-SAFT (WOA) is also analyzed. Finally, the relationship between the binary interaction parameter of the asphaltene-CO$_2$ pair and crossover temperature, below which asphaltene solubility increases in reservoir fluid, with CO$_2$ gas injection is also studied.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
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Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
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Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Modeling of phase equilibrium of North Sea oils with water and MEG

The complex phase equilibrium between reservoir fluids and associating compounds like water and glycols has become very important as the increasing global energy demand pushes the oil industry to use advanced methods to increase oil recovery, such as increasing the use of various chemicals to ensure a constant and safe production. The CPA equation of state has been successfully applied in the past to well defined systems and gas condensates containing associating compounds. It has also been extended to reservoir fluids in presence of water and polar chemicals using modified correlations for critical temperature, pressure and acentric factor. In this work, we evaluate CPA using recently developed correlations for predicting the binary interaction parameters between MEG/hydrocarbons and water/hydrocarbons, for a wide range of systems containing reservoir fluids and production chemicals, such as water and ethylene glycol (MEG). Using these new correlations for prediction of all binary interactions, the CPA EoS satisfactorily describes the mutual solubility of the “binary systems” reservoir fluid and MEG and promising results are also obtained with CPA for ternary mixtures (reservoir fluid + water + MEG), with some deviations for the solubility of hydrocarbons in the polar phase. Improved predictions are observed, when using correlations for binary interactions compared to previous methods of using an average kij fitted to binary data.
Modeling systems relevant to the biodiesel production using the CPA equation of state

In this study, CPA parameters for heavy esters, glycerides, organic acids, and glycerol are presented, together with trends of these parameters against the van der Waals volume. Such trends allow the prediction of parameters for compounds for which data are not available. Pure fluid parameters were estimated by adjusting model predictions to recent DIPPR correlations and carefully selected literature data. Then, the performance of CPA was evaluated in correlating the vapor–liquid equilibrium of binary systems containing fatty acids and their esters, glycerides, water, alcohols and/or glycerol. Satisfactory correlation results were obtained using one (water-acids, alcohols/water - glycerol) or two (systems containing fatty acid esters with water, alcohols or glycerol and mixtures containing glycerides and alcohols) interaction parameters. Moreover, the interaction parameters show smooth trends with carbon chain length, permitting extrapolation for systems for which data are not available. Finally, the estimated parameters and correlations were used for the prediction of liquid-liquid equilibrium of one ternary and one multicomponent mixture. The results showed that accurate predictions are feasible, however indicated the need of more accurate data, at least for important binary mixtures, such as the systems with glycerol.

**General information**

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Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Modelling and control of nitrogen and phosphorus removing systems

General information
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Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Krüger A/S, University of Santiago de Compostela
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Modelling and sensitivity analysis of urinary platinum excretion in anticancer chemotherapy for the recovery of platinum
Platinum (Pt) based antineoplastics are important in cancer therapy. To date the Pt which is urinary excreted by the patients ends up in wastewater. This is disadvantageous from both an economic as from an ecological point of view because Pt is a valuable material and the excretion products are toxic for aquatic organisms. Therefore, efforts should be made to recover the Pt. The urinary excretion of Pt from two antineoplastics are taken under consideration, i.e. cisplatin and carboplatin. Using these reference compounds, a scenario analysis based on administration statistics from Ghent University Hospital in combination with compartmental models for urinary Pt excretion was performed to simulate the average Pt excretion profile during common treatment schemes. These average profiles can be used to assess the technical, social and economic feasibility of Pt-recovery from urine or wastewater. A one-compartment model is used for cisplatin, which is calibrated using the experimental data of six patients. In contrast, a two-compartment model with parameters from literature is used for carboplatin. A Global Sensitivity Analysis revealed kel, the rate constant of elimination, is the most sensitive parameter in the one-compartment model whereas Qu, the urine production rate, was the most sensitive in the two-compartment model for the Pt concentration Cu in urine and the excreted mass of Pt via urine. A GLUE uncertainty analysis showed that all experimental data are within the 95% uncertainty boundaries.

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Modelling and simulation of a U-loop Reactor for Single Cell Protein Production

In this work, two approaches of modelling a one phase U-loop reactor are presented. A simple CSTR model consisting of first-principles dynamic process equations was implemented in Matlab. The results give a good indication of the basic understanding of the effect of changing operation conditions on process performance. For a given product yield, the work investigates how process parameters such as dilution rate (D) or the methanol concentration should be selected to optimize the production. Nevertheless, this simple model exhibits some limitations hindering the development of the optimal operation procedure, such as the impact of the reactor geometry on the operating conditions. Some main hydrodynamic characterization parameters, like the mixing and the mass transfer coefficient kLa are geometry dependent. The second modelling approach attempts to overcome the above-mentioned problems. A three-dimensional one-phase model using Computational Fluid Dynamics (CFD) methods is proposed. By introducing the momentum balances in the simulation, the results can capture the flow velocity fields in three dimensions. It is thereby possible to indicate the influence of the geometric design on the production yield. This methodology allows further research on the effect of design choices on optimal operation, such as the determination of where to locate the substrate input, the static mixer position or the gas injection position.

Modelling and synthesis of pharmaceutical processes: moving from batch to continuous

Research in pharmaceutical process development has gained a lot of interest over the last years. Long development times, increasing R&D costs, increasing competition, and short patent duration are some of the driving forces for the increased research efforts in the field. Increased process understanding of the pharmaceutical process has resulted in major improvements in the field. Process systems engineering (PSE) approaches, which have been successfully applied in the design, analysis and optimization of chemical and petrochemical processes, might be also important for the improvement of pharmaceutical processes by providing systematic and structured solutions for the stages of the pharmaceutical process development.

In this PhD thesis, the objective is to systematize the pharmaceutical process development in order to enhance process understanding by creating a data-rich environment and to investigate/evaluate opportunities for continuous operation. To achieve the mentioned objectives the use of an integrated framework based on systematic model-based methods and tools is proposed. Computer-aided methods and tools are used to generate process knowledge and to evaluate different operational scenarios.

The developed framework is divided into four main sections: the reaction pathway, reaction analysis, separation synthesis and process evaluation-operation based on evaluation. In the first section, the selection of the reaction pathway to produce a desired active ingredient is examined. A reaction database for small pharmaceutical molecules, including
information for reactions, the solvent role and processing information, has been developed to assist the reaction pathway selection. In the second section, the reaction analysis, the identified individual reactions during the reaction pathway selection are analysed. The objective of the reaction analysis section is to collect reaction data and by using model-based methods to investigate possibilities of reaction improvement by evaluating the reaction conditions, the operating mode, the solvent role, and the reactor design. In the third section, alternatives for the separation of the reaction mixture are generated based on the driving force principles and evaluated based on performance criteria, such as mass and energy utilization. Finally, the overall process is simulated and evaluated in terms of productivity and environmental impact. Process optimization studies are performed by defining optimization target based on the process analysis. The application of the developed integrated framework is highlighted through four case studies. In the first case study, the overall use of the framework is highlighted using the synthesis of ibuprofen as a motivating example. The second case study focuses on the application of the developed solvent selection methodology for solvent swap problems. The third case study focused on multiphase reaction systems and improvements through the combination of reaction-separation. Finally, model-based analysis-design is performed for the operation improvement of a glucose isomerization plant.

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Modelling of gas diffusion limitations in Ni/YSZ electrode material in CO2 and co-electrolysis
Carbon formation during CO2 and co-electrolysis (combined electrolysis of H2O and CO2) has been observed in recent studies, under operating conditions where carbon formation based on the bulk gas composition, should be thermodynamically unfavorable. The carbon can principally be formed by the Boudouard reaction (2CO à CO2 + C(s)) or the COreduction reaction (CO+H2 à H2O + C(s)), and will disintegrate the cell structure as it grows. It is therefore of great importance to be able to predict when the carbon is formed, and subsequently take actions to prevent formation. The literature offers suggestions that the carbon formation is caused by diffusion limitations within the Ni/YSZ electrode, but this has not been verified. To do so, the diffusion has been modelled with the dusty gas model and the effect of the electrode tortuosity, porosity, temperature T, electrode thickness dc, and current density i, has been investigated. It is shown that diffusion limitations on reactant transport may lead to very significant increases in equilibrium temperatures for the two carbon forming reactions. For given electrode properties (e, t and dc) increasing current density leads to increasing equilibrium temperatures. The model can be used to calculate limitations on operating conditions (T, i) that ensure no carbon formation.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS
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Modelling of Salt Solubilities for Smart Water flooding in Carbonate Reservoirs using Extended UNIQUAC Model

For most oil reservoirs which were drilled with conventional methods, the expected initial recovery of available hydrocarbons maybe as low as 15% – thus leaving 85+% of hydrocarbons in the reservoir. Implementation of mechanical methods including pump jacks and initial gas injection or thermal recovery can increase that capture up to 25-30% of original oil in place (OOIP). But cost effective Enhanced Oil Recovery (EOR) techniques if implemented correctly can be used to produce another 10-15% of the initially available hydrocarbons.

Advanced water flooding (i.e. altering injection brine compositions by varying concentration of selected ions) is an enhanced oil recovery method which in a low cost, non-toxic manner increases oil recovery from various carbonate reservoirs. Dan and Halfdan are chalk reservoirs from the Danish North Sea, which are mature oil fields that have been flooded with water for more than a decade and are potential candidates for brine composition based EOR. Advanced water flooding through alteration in brine composition has been termed as Smart Water (SmW) Flooding. Designed Water flooding, Low salinity brine injection, LowSal(™) EOR, and Advanced Water flooding in different research studies. Several spontaneous imbibition and water flooding experiments have been conducted in order to understand the fundamental mechanism behind the observed increase in oil recovery for variation in injection of brine composition. When reported in literature, this observed increase in oil recovery has been explained using the wettability alteration mechanism. The wettability alteration mechanism reported in literature can be divided into two parts:

1. Substitution of calcium by magnesium: When Mg containing brine is injected into a core plug, the existing Ca\(^{2+}\) from the mineral surface/lattice is gradually replaced by the injected Mg\(^{2+}\). Decrease in magnesium concentration in the effluent and the corresponding increase in calcium concentration further support this phenomenon.

2. Adsorption of SO\(_4^{2-}\) ions: When SO\(_4^{2-}\) ions are injected into the core plugs along with Ca\(^{2+}\) and/or Mg\(^{2+}\) ions, then SO\(_4^{2-}\) ions get adsorbed on the mineral surface. This leads to desorption of carboxyl ions from the mineral surface and makes the oil more mobile. Thus, eventually leading to an increase in oil recovery. According to the wettability alteration mechanism, an increase in oil recovery therefore takes place when brines with high concentrations of Ca\(^{2+}\), Mg\(^{2+}\), and SO\(_4^{2-}\) ions are injected. It has been further recommended that precipitation of ions must be avoided as precipitation can choke the pore throats and thus have an adverse effect on the sweep efficiency of the flooded water. Several questions have been raised to the wettability alteration mechanism due to fundamental contradictions with experiments. It has been observed that Stevns Klint chalk from Denmark shows consistent increase in oil recovery for an increase in injection brine SO\(_4^{2-}\) concentration. But similar increases in oil recovery are not observed for Niobrara or Rørdal outcrop chalk core plugs.

Observed increases in oil recovery for completely water wet core plugs are also contradictory to the proposed wettability alteration mechanism. No increase in oil recovery observed when injecting brines with high concentrations of SO\(_4^{2-}\) ions is also contradictory to the proposed wettability alteration mechanism. Therefore, understanding the fundamental mechanism behind SmW-EOR is quite important. In this study it is attempted to conduct geochemical modelling of salt solubility at reservoir conditions to explore the possible correlation between different brine properties and the corresponding increase in oil recovery (as reported in literature).

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Modelling of volumetric composition and mechanical properties of unidirectional hemp/epoxy composites - Effect of enzymatic fibre treatment

The objective of the present study is to assess the effect of enzymatic fibre treatments on the fibre performance in unidirectional hemp/epoxy composites by modelling the volumetric composition and mechanical properties of the composites. It is shown that the applied models can well predict the changes in volumetric composition and mechanical properties of the composites when differently treated hemp fibres are used. The decrease in the fibre correlated porosity factor with the enzymatic fibre treatments shows that the removal of pectin by pectinolytic enzymes results in a better fibre
Impregnation by the epoxy matrix, and the mechanical properties of the composites are thereby increased. The effective fibre stiffness and strength established from the modelling show that the enzymatic removal of pectin also leads to increased mechanical properties of the fibres. Among the investigated samples, the composites with hydrothermally pre-treated and enzymatically treated fibres have the lowest porosity factor of 0.08 and the highest mechanical properties. In these composites, the effective fibre stiffness and strength are determined to be 83 GPa and 667 MPa, respectively, when the porosity efficiency exponent is set equal to 2. Altogether, it is demonstrated that the applied models provide a concept to be used for the evaluation of performance of treated fibres in composites.

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**Modelling phase equilibria for acid gas mixtures using the CPA equation of state. Part VI. Multicomponent mixtures with glycols relevant to oil and gas and to liquid or supercritical CO₂ transport applications**
In this work the Cubic Plus Association (CPA) equation of state is applied to multicomponent mixtures containing CO₂ with alkanes, water, and glycols. Various modelling approaches are used i.e. different association schemes for pure CO₂ (assuming that it is a non-associating compound, or that it is a self-associating fluid with two, three or four association sites) and different possibilities for modelling mixtures of CO₂ with other hydrogen bonding fluids (only use of one interaction parameter kij or assuming cross association interactions and obtaining the relevant parameters either via a combining rule or using an experimental value for the cross association energy). Initially, new binary interaction
parameters were estimated for (CO$_2$ + glycol) binary mixtures. Having the binary parameters from the binary systems, the model was applied in a predictive way (i.e. no parameters were adjusted to data on ternary and multicomponent mixtures) to model the phase behaviour of ternary and quaternary systems with CO$_2$ and glycols. It is concluded that CPA performs satisfactorily for most multicomponent systems considered. Some differences between the various modelling approaches are observed. This work is the last part of a series of studies, which aim to arrive in a single "engineering approach" for applying CPA to acid gas mixtures, without introducing significant changes to the model. An overall assessment, based also on the obtained results of this series (Tsivintzelis et al., 2010, 2011, 2014, 2015, 2015), which is based on an investigation of about 30 multicomponent systems containing acid gases, water, alcohols, glycols and hydrocarbons, reveals that assuming cross association (solvation) of CO$_2$ with glycols, alcohols and water or alternatively considering CO$_2$ to be a self-associating molecule (with three or four sites) are the better approaches which perform similarly and quite satisfactorily. However, the use of the former one (solvation), using whenever possible experimental values for the cross association energy, in all cases is recommended.

**General information**

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Scopus rating (2008): SJR 1.414 SNIP 1.269
Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes

This paper proposes a series of extensions to functionally upgrade the IWA Anaerobic Digestion Model No. 1 (ADM1) to allow for plant-wide phosphorus (P) simulation. The close interplay between the P, sulfur (S) and iron (Fe) cycles requires a substantial (and unavoidable) increase in model complexity due to the involved three-phase physico-chemical and biological transformations. The ADM1 version, implemented in the plant-wide context provided by the Benchmark Simulation Model No. 2 (BSM2), is used as the basic platform (A0). Three different model extensions (A1, A2, A3) are implemented, simulated and evaluated. The first extension (A1) considers P transformations by accounting for the kinetic decay of polyphosphates (XPP) and potential uptake of volatile fatty acids (VFA) to produce polyhydroxyalkanoates (XPHA) by phosphorus accumulating organisms (XPAO). Two variant extensions (A2,1/A2,2) describe biological production of sulfides (SIS) by means of sulfate reducing bacteria (XSRB) utilising hydrogen only (autolithotrophically) or hydrogen plus organic acids (heterorganotrophically) as electron sources, respectively. These two approaches also consider a potential hydrogen sulfide (ZH2S) inhibition effect and stripping to the gas phase (GH2S). The third extension (A3) accounts for chemical iron (III) (SFe 3+) reduction to iron (II) (SFe 2+) using hydrogen (SH2) and sulfides (SIS) as electron donors. A set of pre/post interfaces between the Activated Sludge Model No. 2d (ASM2d) and ADM1 are furthermore proposed in order to allow for plant-wide (model-based) analysis and study of the interactions between the water and sludge lines. Simulation (A1 - A3) results show that the ratio between soluble/particulate P compounds strongly depends on the pH and cationic load, which determines the capacity to form (or not) precipitation products. Implementations A1 and A2,1/A2,2 lead to a reduction in the predicted methane/biogas production (and potential energy recovery) compared to reference ADM1 predictions (A0). This reduction is attributed to two factors: (1) loss of electron equivalents due to sulfate (SSO4) reduction by XSRB and storage of XPHA by XPAO; and, (2) decrease of acetoclastic and hydrogenotrophic methanogenesis due to ZH2S inhibition. Model A3 shows the potential for iron to remove free SIS (and consequently inhibition) and instead promote iron sulfide (XFeS) precipitation. It also reduces the quantities of struvite (XMgNH4PO4) and calcium phosphate (XCa3(PO4)2) that are formed due to its higher affinity for phosphate anions. This study provides a detailed analysis of the different model assumptions, the effect that operational/design conditions have on the model predictions and the practical implications of the proposed model extensions in view of plant-wide modelling/development of resource recovery strategies.

General information
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BFI (2012): BFI-level 2
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.582 SNIP 2.196
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.319 SNIP 2.225
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Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.994 SNIP 2.208
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Modelling the phase equilibria of multicomponent mixtures containing \( \text{CO}_2 \), alkanes, water, and/or alcohols using the quadrupolar CPA equation of state

In this work, a quadrupolar cubic plus association (qCPA) equation of state is evaluated for its ability to predict the phase equilibria of multicomponent mixtures containing \( \text{CO}_2 \) and alkanes, alcohols, and/or water. A single binary interaction parameter is employed in qCPA for all binary combinations. All parameters are based solely on pure fluid or binary mixture data and multicomponent data are used only to evaluate the predictions. The performance of qCPA is, for all mixtures, compared to CPA where \( \text{CO}_2 \) is considered to be either non-associating (inert), solvating or self-associating. In the latter two approaches, an additional adjustable parameter is employed for binary pairs of \( \text{CO}_2 \) and an associating compound. The results show that the predictions with qCPA are very similar to the best performing CPA approaches, even though the model uses fewer adjustable binary parameters. The predictions with qCPA and the best CPA approaches are typically satisfactory and predict the general behaviour of the systems. As expected, qCPA and CPA with solvation or association typically performs better than inert CPA for two- and three phase vapour–liquid and vapour–liquid–liquid equilibria. However, inert CPA yields the best results of all the models for the prediction of dew point pressures.
Models and Modelling Tools for Chemical Product and Process Design

The design, development and reliability of a chemical product and the process to manufacture it, need to be consistent with the end-use characteristics of the desired product. One of the common ways to match the desired product-process characteristics is through trial and error based experiments, which can be expensive and time consuming. An alternative approach is the use of a systematic model-based framework according to an established work-flow in product-process design, replacing some of the time consuming and/or repetitive experimental steps. The advantages of the use of a model-based framework is that in the design, development and/or manufacturing of a chemical product-process, the knowledge of the applied phenomena together with the product-process design details can be provided with diverse degrees of abstractions and details. This would allow the experimental resources to be employed for validation and fine-tuning of the solutions from the model-based framework, thereby, removing the need for trial and error experimental steps. Also, questions related to economic feasibility, operability and sustainability, among others, can be considered in the early stages of design. However, are the needed models for such a framework available? Or, are modelling tools that can help to develop the needed models available? Can such a model-based framework provide the needed model-based workflows matching the requirements of the specific chemical product-process design problems? What types of models are needed for innovative and more sustainable design? The presentation will review the current state of the art in models and modelling tools suitable for chemical product-process design and point out the gaps that need to be filled out with respect to model-based frameworks for chemical product-process design. Illustrative examples highlighting the need for efficient model-based systems will be presented, where the need for predictive models for innovative chemical product-process design will be highlighted. The examples will cover aspects of chemical product-process design where the idea of the grand chemical product design model, that also incorporates the process design issues together with sustainability issues will be presented.

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Editors: Kravanja, Z., Bogataj, M.
Molecular and biochemical characterization of a new thermostable bacterial laccase from *Meiothermus ruber* DSM 1279

A new laccase gene (*mrlac*) from *Meiothermus ruber* DSM 1279 was successfully overexpressed to produce a laccase (Mrlac) in soluble form in *Escherichia coli* during simultaneous overexpression of a chaperone protein (GroEL/ES). Without the GroEL/ES protein, the Mrlac overexpressed in *E. coli* constituted a huge amount of the total cellular protein, but the enzyme was localized in the insoluble fraction with no activity in the soluble fraction. Co-expression of the Mrlac with the *E. coli* GroEL/ES drastically improved proper folding and expression of active Mrlac in the soluble fraction. Spectroscopic analysis of the purified enzyme by UV/visible and electron paramagnetic resonance spectroscopy confirmed that the Mrlac was a multicopper oxidase. The Mrlac had a molecular weight of ~50 kDa and exhibited activity towards the canonical laccase substrates 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid) (ABTS), syringaldazine (SGZ), and 2,6-dimethoxyphenol (2,6-DMP). Kinetic constants $K_m$ and $k_{cat}$ were 27.3 µM and 325 min$^{-1}$ on ABTS, 4.2 µM and 106 min$^{-1}$ on SGZ, and 3.01 µM and 115 min$^{-1}$ on 2,6-DMP, respectively. Maximal enzyme activity was achieved at 70°C with ABTS as substrate. In addition, Mrlac exhibited a half-life for deactivation at 70°C and 75°C of about 120 min and 67 min, respectively, indicating that the Mrlac is intrinsically thermostable. Finally, Mrlac was efficient in catalyzing the removal of 2,4-dichlorophene (DCP) in aqueous solution, a trait which makes the enzyme potentially useful for environmentally friendly applications.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Kalyani, D. C. (Intern), Munk, L. (Intern), Mikkelsen, J. D. (Intern), Meyer, A. S. (Intern)
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- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
Molecular beam deposition of high-permittivity polydimethylsiloxane for nanometer-thin elastomer films in dielectric actuators

To realize low-voltage dielectric elastomer actuators (DEAs) for artificial muscles, a high-permittivity elastomer and a related thin-film deposition technique must be selected. For polydimethylsiloxane, fillers or functionalized crosslinkers have been incorporated into the elastomer to improve dielectric properties. To produce elastomer layers nanometers thin, molecular beam deposition was introduced. We pursue the synthesis of a high-permittivity oligomer, namely a chloropropyl-functional, vinyl-terminated siloxane to be thermally evaporated and subsequent UV curing to form an elastomer. The synthesized oligomer exhibits dielectric permittivity enhanced by 33% and a breakdown increase of 26% with respect to the commercially available oligomer DMS-V05. Films 160 nm thin were fabricated after being evaporated under ultra-high vacuum conditions. Spectroscopic ellipsometry served for film growth monitoring. Using atomic force microscopy, the film surface morphology and mechanics were characterized after growth termination and subsequent curing. The Young's modulus of the elastomer corresponded to $(1.8 \pm 0.2) \text{ MPa}$ and is thus a factor of two lower than that of DMS-V05. Consequently, the properties of the films prepared by the new elastomer can be quantified by the normalized figure of merit, which estimates to 4.6. The presented approach is an essential step toward the realization of low-voltage DEA for medical applications and beyond.
Monolithic PDMS Laminates for Dielectric Elastomer Transducers through Open-Air Plasma Treatment

The present study investigates the use of an open-air plasma-treatment system for the surface modification of polydimethylsiloxane (PDMS), in order to improve layer-to-layer adhesion. The procedure presented herein is more cost efficient compared to conventional vacuum-based plasma-treatment, and it is performed at different speeds and distances away from the nozzle, to investigate how these two parameters influence the resulting interfacial layer of two fully cured PDMS films. The plasma-treatment is determined not to alter mechanical properties compared to the single film, while peel forces are sufficient to avoid delamination during operation.

General information
State: Published
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Pages: 769-774
Publication date: 2016
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.389 SNIP 0.57 CiteScore 1.34
Understanding the mechanism of fracture is essential for material and process design. While the initiation of fracture in brittle solids is generally associated with the preexistence of material imperfections, the mechanism for initiation of fracture in viscoelastic fluids, e.g., polymer melts and solutions, remains an open question. We use high speed imaging to visualize crack propagation in entangled polymer liquid filaments under tension. The images reveal the simultaneous propagation of multiple cracks. The critical stress and strain for the onset of crack propagation are found to be highly reproducible functions of the stretch rate, while the position of initiation is completely random. The reproducibility of conditions for fracture points to a mechanism for crack initiation that depends on the dynamic state of the material alone, while the crack profiles reveal the mechanism of energy dissipation during crack propagation.
Multivariable Optimization of the Piperazine CO2 Post-Combustion Process

8 molal piperazine (PZ) is a promising solvent for developing an energy efficient CO2 post-combustion capture process. However, it has a limited operating range due to precipitation. The operating range can be extended by decreasing the piperazine concentration and/or increasing the CO2 loading of the lean solvent. However, optimal solvent composition must be determined taking into account the solvent circulation rate and the heat demand of the solvent regeneration. In this paper, we determine and generalize trends of performance for a broad range of operating conditions: 1.8 to 9 mol PZ/kg water, 0.2 to 0.6 lean loading, and for two flue gas sources: natural gas combined cycle power plant (NGCC, 3.9 mol% CO2) and a coal based power plant (ASC, 13.25 mol% CO2). Special attention is given to the boundaries where precipitation may occur. The results are created by the hybrid CAPCO2 rate-based model which accounts for precipitation when estimating the heat and mass transfer rates. The results show that the 7 molal piperazine gives the lowest specific reboiler duty at 0.40 CO2 lean loading: 3.32 GJ/t CO2 and 4.05 GJ/t CO2 for the ASC case and NGCC cases. The analysis also reveals that the capture process needs to be operated up to 7.8% above the minimum duty to avoid the risk of clogging due to solid formation. Note, this analysis assumes a 25°C minimum solvent temperature. The energy requirement of the capture process can be further improved by assuming a minimum solvent temperature of 30°C which gives a specific reboiler duty of 3.23 GJ/t CO2 (ASC case) and 3.80 GJ/t CO2 (NGCC case).
Nematic effects and strain coupling in entangled polymer melts under strong flow

We use small-angle neutron scattering (SANS) to study labeled short chains with and without the influence of an entangled and highly stretched surrounding environment of longer chains. We find unequivocal evidence of nematic effects as the blend chains in steady state flow are stretched a factor \( \sim 1.5 \) more from the presence of the long chain nematic field. In the pure melt we confirm that the nonaffine mean-field result \( \nu = 0.5 \) for the strain coupling is still valid for very fast flows, while in the nematic system our analysis predicts an increased coupling constant. We provide a structural explanation for the two first regimes of the nonlinear relaxation, particularly a transition regime where the long chains are relaxing in a sea of reptating short chains.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Micro- and Nanotechnology, Amphiphilic Polymers in Biological Sensing, University of Copenhagen, Australian Nuclear Science and Technology Organisation
Authors: Kirkensgaard, J. J. K. (Ekstern), Hengeller, L. (Intern), Dorokhin, A. (Intern), Huang, Q. (Intern), Garvey, C. J. (Ekstern), Almdal, K. (Intern), Hassager, O. (Intern), Mortensen, K. (Intern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.22 SNIP 1.123 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.311 SNIP 1.239 CiteScore 2.28
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Neutral lipid production in Dunaliella salina during osmotic stress and adaptation

The salt-tolerant green microalga Dunaliella salina can survive both hyper- and hypo-osmotic shock. Upon osmotic shock, the cells transiently and rapidly decreased or increased in size within minutes and slowly over hours acquired their original cell size and volume. Cell size distribution differs significantly in the cultures grown in the salinity range from 1.5 to 15 % NaCl. By using Nile Red fluorescence to detect neutral lipids, it became clear that only hyper-osmotic shock on cells induced transient neutral lipid appearance in D. salina, while those transferred from 9 to 15 % NaCl stimulated the most neutral lipid accumulation. These cells grew well in 9 % NaCl, but they cannot recover a shift to 15 % NaCl and cell division is accordingly slowed down. The transient appearance of neutral lipid could be dependent on the inhibition of cell division experiencing the NaCl shift. Moreover, the effect of nutrient limitation slows down cell division and photosynthesis as a secondary result, which triggers the cells to accumulate neutral storage lipids when they entered the stationary phase, which is seen in all the batch cultures of D. salina grown in the salinity range of 3–15 %. The changes in salt concentration did not significantly influence the overall fatty acid composition in D. salina cells. Although there shows both increased amounts of total lipids and neutral lipids in the cells grown in salinity higher than 9 % NaCl, lipid productivity is however compromised by the slower cell growth rate and lower cell density under this condition.
**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Shenyang Agricultural University
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- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.46
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): CiteScore 2.32
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): CiteScore 2.88
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): CiteScore 2.78
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): CiteScore 2.68
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): CiteScore 2.29
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
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New Realization of Periodic Cycled Separation

A new realization of periodic cycled gas/liquid separation is presented. Separation factors and column efficiencies are compared for a column stripping ammonia from water with air, using three different sets of internals: conventional sieve trays, Sulzer BX gauze packings, and periodically cycled trays. The proposed new periodic trays are shown to be advantageous compared to their continuous alternatives. It is demonstrated experimentally that periodic tray efficiencies of up to 300% are achievable. With the proposed new tray design, a new operation form is also introduced in which the trays are drained sequentially rather than simultaneously, such that the vapor flow is not interrupted during the liquid drainage. For different ratios of counter-current vapor/liquid flow rates, column efficiencies for periodically cycled columns are shown experimentally to be two times greater than those for columns with sieve trays.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
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Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
New Vistas in Chemical Product and Process Design

Design of chemicals-based products is broadly classified into those that are process centered and those that are product centered. In this article, the designs of both classes of products are reviewed from a process systems point of view; developments related to the design of the chemical product, its corresponding process, and its integration are highlighted. Although significant advances have been made in the development of systematic model-based techniques for process design (also for optimization, operation, and control), much work is needed to reach the same level for product design. Timeline diagrams illustrating key contributions in product design, process design, and integrated product-process design are presented. The search for novel, innovative, and sustainable solutions must be matched by consideration of issues related to the multidisciplinary nature of problems, the lack of data needed for model development, solution strategies that incorporate multiscale options, and reliability versus predictive power. The need for an integrated model-experiment-based design approach is discussed together with benefits of employing a systematic computer-aided framework with built-in design templates.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Zhang, L. (Intern), Babi, D. K. (Intern), Gani, R. (Intern)
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Web of Science (2016): Indexed yes
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NLP modeling for the optimization of LiBr-H2O absorption refrigeration systems with exergy loss rate, heat transfer area, and cost as single objective functions

Based on a nonlinear mathematical programming model, the sizes and operating conditions of the process units of single-effect absorption refrigeration systems operating with a LiBr–H2O solution are optimized for a specified cooling capacity by minimizing three single objective functions: the total exergy loss rate, the total heat transfer area, and the total annual cost of the system. It was found that the optimal solution obtained by minimization of the total exergy loss rate provides “theoretical” upper bounds not only for the total heat transfer area of the system but also for each process unit and all stream temperatures, while the optimal solution obtained by minimization of the total heat transfer area provides the lower bounds for these model variables, to solve a cost optimization problem. The minimization of the total exergy loss rate by varying parametrically the available total heat transfer area between these bounds was also performed, allowing to see how the optimal distribution of the available total heat transfer area among the system components, as well as the operating conditions (stream temperature, pressure, composition, and mass flow rate) and heat loads, vary qualitatively and quantitatively with increasing available total heat transfer area. These optimization results allowed to find a “practical” value of the total heat transfer area, i.e. no benefits can be obtained by increasing the available total heat transfer area above this value since the minimal total exergy loss value cannot be significantly improved by distributing additional heat transfer area among the process units. The optimal solution corresponding to this practical value significantly improves the upper bounds for an economic optimization problem with respect to the optimal solution corresponding to the theoretical value. The optimal solutions corresponding to the theoretical and the practical upper bound values for the total heat transfer area (100 m² and 61 m², respectively) as well as the optimal solution obtained by minimization of the total annual cost are discussed for a case study considering a cooling capacity of 50 kW, upon the model assumptions made and a given cost model.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Tecnologica Nacional Facultad Regional Rosario, Technische Universität Berlin
Authors: Mussati, S. F. (Ekstern), Gernaey, K. (Intern), Morosuk, T. (Ekstern), Mussati, M. C. (Intern)
Pages: 526-544
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Scopus rating (2016): CiteScore 6.04 SJR 2.287 SNIP 2.065
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.09 SNIP 2.092 CiteScore 5.24
Web of Science (2015): Indexed yes
Novel high dielectric constant hybrid elastomers based on glycerol-insilicone emulsions

Novel hybrid elastomers were prepared by speedmixing of two virtually immiscible liquids – glycerol and polydimethylsiloxane (PDMS) prepolymer. Upon crosslinking of the PDMS phase of the resulting glycerol-in-silicone emulsion freestanding films were obtained. In this way glycerol became uniformly distributed within PDMS in shape of discrete droplets thus acting as a high dielectric constant filler efficiently enhancing the dielectric constant of the composites. Low- and high-voltage dielectric spectroscopy measurements were conducted in order to verify applicability of the composites as dielectric elastomer actuators. Conductivities of samples based on various PDMS compositions with different loadings of embedded glycerol were thoroughly investigated providing useful information about the dielectric behavior.
Novel strategies for control of fermentation processes

There is increasing interest in applying more advanced control strategies to biological processes in order to optimise the operation of these complex systems. In the past years, the major increases in product titre have been achieved mainly by genetic engineering approaches, which has lead to highly optimised industrial host strains. The focus of this project is instead on en-gineering of the process. The question to be answered in this thesis is, given a highly optimised industrial host strain, how can we operate the fermentation process in order to maximise the productivity of the system?

In order to develop control strategies a significant effort must be invested into developing process models and establishing process understanding. Both data-driven modelling and mechanistic modelling approaches are considered in this work. Firstly, multivariate analysis is applied to production scale data from Novozymes A/S in order to predict the product concentration which is measured at the end of the batch. This is achieved with an average prediction error of 7.4%. The purpose of developing the model, is mainly in order to identify key process parameters which show variance relevant to the product concentration, and to identify process trends which lead to higher titres. The application of multivariate methods, in order to provide process insights, creates value from the vast datasets which are collected in industry.

A mechanistic model approach is then considered, based on previous work by Albaek et al (2012). This model describes the fungal processes operated in the fermentation pilot plant at Novozymes A/S. This model is investigated using uncertainty analysis methods in order to assess the applicability to control applications. A mechanistic model approach is desirable, as it is a predictive method which is able to be extrapolated outside of the conditions used to develop the model.

For this reason, the mechanistic model approach is further investigated in this work. The mechanistic model analysis showed that it provided a robust description of the physical system, however there was a relatively high uncertainty in the description of the biological processes. For control applications the model is applied online, and therefore it is investigated whether the model prediction may be improved by incorporating available measurement data. A stoichiometric balance approach is applied in order to estimate model parameters including the rate of biomass formation and the rate of product formation. This leads to an increased prediction accuracy in the biological part of the model. The mechanistic model may then be applied as a valuable on-line monitoring tool.

The control strategy development follows on from the on-line model application. The aim of the control strategy is to maximise the total product achieved per batch. There is a demand to maximise the total product in each batch in industry, in order to meet increasing product demands with a limited capacity. The control algorithm is then defined in order to maximise the mass in the system, subject to the oxygen transfer rates in the system. Since the aim is to control to a target fill in a target time, a predictive model-based control algorithm is developed where by the model is simulated to the end of batch time at each model iteration. This provides a prediction of the future trajectory of the process, so that it is possible to guide the system to the desired target mass. The control strategy is applied on-line at 550L scale in the Novozymes A/S fermentation pilot plant, and the method is challenged with four different sets of process operating conditions. The controller reliably reaches the desired maximum tank fill, with a maximum error of under 5% of the target in eight experimental runs. The product concentration is not affected by the control strategy when compared to batches utilising a reference controller. This method has the benefit of reducing the variance in the final fill, which not only allows for a more reproducible product mass in a batch operation, but also aids downstream process scheduling and resource allocation activities in the industrial setting.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Novozymes A/S
Authors: Mears, L. (Intern), Gernaey, K. (Intern), Sin, G. (Intern), Stocks, S. (Ekstern), Cassells, B. (Ekstern)
Number of pages: 149
Publication date: 2016
Novel α-L-Fucosidases from a Soil Metagenome for Production of Fucosylated Human Milk Oligosaccharides

This paper describes the discovery of novel α-L-fucosidases and evaluation of their potential to catalyse the transglycosylation reaction leading to production of fucosylated human milk oligosaccharides. Seven novel α-L-fucosidase-encoding genes were identified by functional screening of a soil-derived metagenome library and expressed in E. coli as recombinant 6xHis-tagged proteins. All seven fucosidases belong to glycosyl hydrolase family 29 (GH 29). Six of the seven α-L-fucosidases were substrate-inhibited, moderately thermostable and most hydrolytically active in the pH range 6-7, when tested with para-nitrophenyl-α-L-fucopyranoside (pNP-Fuc) as the substrate. In contrast, one fucosidase (Mfuc6) exhibited a high pH optimum and an unusual sigmoidal kinetics towards pNP-Fuc substrate. When tested for trans-fucosylation activity using pNP-Fuc as donor, most of the enzymes were able to transfer fucose to pNP-Fuc (self-condensation) or to lactose. With the α-L-fucosidase from Thermotoga maritima and the metagenome-derived Mfuc5, different fucosyllactose variants including the principal fucosylated HMO 2'-fucosyllactose were synthesised in yields of up to ~6.4%. Mfuc5 was able to release fucose from xyloglucan and could also use it as a fucosyl-donor for synthesis of fucosyllactose. This is the first study describing the use of glycosyl hydrolases for the synthesis of genuine fucosylated human milk oligosaccharides.
Online analysis of oxygen inside silicon-glass microreactors with integrated optical sensors

A powerful online analysis set-up for oxygen measurements within microfluidic devices is presented. It features integration of optical oxygen sensors into microreactors, which enables contactless, accurate and inexpensive readout using commercially available oxygen meters via luminescent lifetime measurements in the frequency domain (phase shifts). The fabrication and patterning of sensor layers down to a size of 100 μm in diameter is performed via automated airbrush spraying and was used for the integration into silicon-glass microreactors. A novel and easily processable sensor material is also presented and consists of a polystyrene- silicone rubber composite matrix with embedded palladium(II) or platinum(II) meso-tetra(4-fluorophenyl) tetrabenzo(N4-phenylporphyrin (PdTPTBPF and PtTPTBPF) as oxygen sensitive dye. The resulting sensor layers have several advantages such as being excitable with red light, emitting in the near-infrared spectral region, being photostable and covering a wide oxygen concentration range. The trace oxygen sensor (PdTPTBPF) in particular shows a resolution of 0.06-0.22 hPa at oxygen concentrations lower than 20 hPa (<2% oxygen) and the normal range oxygen sensor (PtTPTBPF) shows a resolution of 0.2-0.6 hPa at low oxygen concentrations (<50 hPa) and 1-2 hPa at ambient air oxygen concentrations. The sensors were integrated into different silicon-glass microreactors which were manufactured using mass production compatible processes. The obtained microreactors were applied for online monitoring of enzyme transformations, including d-alanine or d-phenylalanine oxidation by d-amino acid oxidase, and glucose oxidation by glucose oxidase.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, IX-factory GmbH, Graz University of Technology
Authors: Ehgartner, J. (Ekstern), Sulzer, P. (Ekstern), Burger, T. (Ekstern), Kasjanow, A. (Ekstern), Bouwes, D. (Ekstern), Krühne, U. (Intern), Klimant, I. (Ekstern), Mayr, T. (Ekstern)
Pages: 748-757
Operation and Design of Diabatic Distillation Processes

Diabatic operation of a distillation column implies that heat is exchanged in one or more stages in the column. The most common way of realising diabatic operation is by internal heat integration resulting in a heat-integrated distillation column (HIDiC). When operating the rectifying section at a higher pressure, a driving force for transferring heat from the rectifying section to the stripping section is achieved. As a result, the condenser and reboiler duties can be significantly reduced. For two-product distillation, the HIDiC is a favourable alternative to the conventional distillation column. Energy savings up to 83% are reported for the HIDiC compared to the CDiC, while the reported economical savings are as high as 40%. However, a simpler heat-integrated distillation column configuration exists, which employs compression in order to obtain a direct heat integration between the top vapour and the reboiler. This configuration is called the mechanical vapour recompression column (MVRC). Energy and economic savings of similar magnitude as the HIDiC are reported for the MVRC. Hence, it is important to develop methods and tools for assisting the selection of the best distillation column configuration. The contributions of this work can be divided in three parts. The first part involves the identification of the preferred distillation column configuration (CDiC, MVRC, or HIDiC) for a given mixture to be separated. Correlations between physical parameters, distillation column design variables, and preliminary feasibility indicators are investigated through simulations studies. The simulation studies include case studies, where different mixtures are separated in different distillation column configurations. The considered mixtures are industrially relevant and their thermodynamic behaviours vary considerably from one another. The HIDiC was found to be the preferred configuration in terms of operating expenditures for mixtures of normal boiling point differences below 10K. The second part involves the investigation of the technological feasibility of the HIDiC. The impact on the column capacity (required tray area, entrainment flooding, weeping) of different column arrangements of the internal heat transfer is investigated. Furthermore, the ability to achieve stable operation of a concentric HIDiC is investigated by systematically designing a regulatory control layer and a supervisory control layer. Stable operation, in terms of column capacity and set point tracking, is demonstrated by simulation. The final part covers the developed simulation tools and methods. A new distillation column model is presented in a generic form such that all the considered distillation column configurations can be described within the same model framework. The following distillation column configurations are considered:

- The conventional distillation column (CDiC)
- The mechanical vapour recompression column (MVRC)
- The heat-integrated distillation column (HIDiC)
- The secondary reflux and vaporisation column (SRVC)

The generic nature of the modelling framework is favourable for benchmarking distillation column configurations. To further facilitate benchmarking of distillation column configurations, a conceptual design algorithm was formulated, which systematically addresses the selection of the design variables. The conceptual design of the heat-integrated distillation column configurations is challenging as a result of the increased number of decision variables compared to the CDiC. Finally, the model is implemented in Matlab and a database of the considered configurations, case studies, pure component properties, and binary interaction parameters is established.
Optimal aigal cultivation for used water resource recovery

General information
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Optimal Operation and Stabilising Control of the Concentric Heat-Integrated Distillation Column
A systematic control structure design method is applied on the concentric heat integrated distillation column (HIDIC) separating benzene and toluene. A degrees of freedom analysis is provided for identifying potential manipulated and controlled variables. Optimal operation is mapped and active constraints are identified for constructing the supervisory control layer. The fundamental problem of obtaining a stabilising control structure is addressed resulting in the regulatory control layer design. A supervisory control layer is devised and combined with the regulatory control layer. The control structure is finally evaluated by dynamic simulation for proving an acceptable performance. (C) 2016, IFAC (International Federation of Automatic Control) Hosting by Elsevier Ltd. All rights

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Optimization of a new flow design for solid oxide cells using computational fluid dynamics modelling
Design of a gas distributor to distribute gas flow into parallel channels for Solid Oxide Cells (SOC) is optimized, with respect to flow distribution, using Computational Fluid Dynamics (CFD) modelling. The CFD model is based on a 3d geometric model and the optimized structural parameters include the width of the channels in the gas distributor and the area in front of the parallel channels. The flow of the optimized design is found to have a flow uniformity index value of 0.978. The effects of deviations from the assumptions used in the modelling (isothermal and non-reacting flow) are evaluated and it is found that a temperature gradient along the parallel channels does not affect the flow uniformity,
whereas a temperature difference between the channels does. The impact of the flow distribution on the maximum obtainable conversion during operation is also investigated and the obtainable overall conversion is found to be directly proportional to the flow uniformity. Finally the effect of manufacturing errors is investigated. The design is shown to be robust towards deviations from design dimensions of at least ±0.1 mm which is well within obtainable tolerances.

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Optimizing integrated reference cases in the OCTAVIUS project

Adding a carbon capture plant to a power plant reduces the efficiency of said power plant. In order to keep this drop in efficiency as small as possible, several optimisation studies are performed in the OCTAVIUS project. Based on the work of the European Benchmarking Task Force-EBTF within the CESAR, CAESAR, and DECARBit projects, two reference power plants are modelled in Ebsilon® Professional. The first is an 800 MWe coal case, the second a 430 MWe natural gas combined cycle (NGCC) case. For each power plant two separate capture plants are considered: one using 30 wt% MEA as solvent system, the other with CESAR1, a mixture of AMP and PZ as solvent system. This results in four different reference cases which are optimized by varying different process parameters and evaluating process modifications. In a second step, the integration of the capture plant into the power plant is evaluated. This is important especially for the coal fired power plant, where integration of waste heat from the capture plant or the CO₂ compressor intercoolers can lead to a significant increase in overall efficiency. The configuration of intercoolers for the CO₂ compressor is adapted to achieve the highest overall efficiency. For the natural gas combined cycle plant, integration is not that beneficial, since there is no heat sink available in the water steam cycle. In the end, the cost of electricity and cost of CO₂ avoided is calculated for all four cases. While the CESAR1 solvent system in a conventional absorber-stripper scheme is less costly (almost 17%) than the MEA solvent system in a process with Lean Vapour Compression for the coal cases, the result is the opposite for the two NGCC cases though the difference is not substantial.

General information
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Oscillatory squeeze flow for the study of linear viscoelastic behavior

The squeezing of a sample between parallel plates has been used for many years to characterize the rheological behavior of soft, purely viscous materials, and in recent times, small-amplitude oscillatory squeezing has been proposed as a means to determine the linear viscoelastic properties of molten polymers and suspensions. The principal advantage of squeeze flow rheometer over rotational devices is the simplicity of the apparatus. It has no air bearing and is much less expensive and easier to use. Accuracy may be somewhat reduced, but for quality control purposes, it could be quite useful. It might also find application as the central component of a high-throughput rheometer for evaluating experimental materials. The deformation is not simple shear, but equations have been derived to show that the oscillatory compressive (normal) force that is measured can serve as a basis for calculating the storage and loss moduli. These theories as well as instruments that have been developed to generate the required deformation are described, and applications to a variety of materials are described.

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Oxidation of lignin in hemp fibres by laccase: effects on mechanical properties of hemp fibres and unidirectional fibre/epoxy composites
PCR-Based Seamless Genome Editing with High Efficiency and Fidelity in *Escherichia coli*

Efficiency and fidelity are the key obstacles for genome editing toolboxes. In the present study, a PCR-based tandem repeat assisted genome editing (TRAGE) method with high efficiency and fidelity was developed. The design of TRAGE is based on the mechanism of repair of spontaneous double-strand breakage (DSB) via replication fork reactivation. First, cat-sacB cassette flanked by tandem repeat sequence was integrated into target site in chromosome assisted by Red enzymes. Then, for the excision of the cat-sacB cassette, only subculturing is needed. The developed method was successfully applied for seamlessly deleting, substituting and inserting targeted genes using PCR products. The effects of different manipulations including sucrose addition time, subculture times in LB with sucrose and stages of inoculation on the efficiency were investigated. With our recommended procedure, seamless excision of cat-sacB cassette can be realized in 48 h efficiently. We believe that the developed method has great potential for seamless genome editing in *E. coli*.

General information
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In recent years, utilization of fats and oils has started to shift towards the bioindustry making them one of the most important renewable materials for the future chemical industry, and leading to oils and fats industry expansion along with a scale reorientation from local to large scale industry [1]. Such developments have led to new challenges regarding the design and development of better performing processes and products. Despite the advances in property modelling and process design techniques available via different computer aided methods and tools for the chemical and petrochemical industries, the oleochemical industry is not able to exploit this knowledge due to a lack of experimental data and property models within commercial software applications and the ability to describe accurately the phase behaviour of systems with lipids. Over the past years, new methods and models for predicting single properties and temperature dependent properties (e.g. critical properties [2], viscosity [3], heat capacity [4], heat of vaporization [4], [5], vapour pressure [5]) have been reported. Likewise, another important modelling task is phase equilibria prediction which is directly related to process synthesis, modelling and simulation. An important aspect in phase equilibria prediction is represented by quality of the data used for regression of model parameters. In previous work, Cunico et al. [5] applied several consistency tests for VLE data sets involving lipids that are available in open literature and their results show that only 3% of the analysed data sets have quality factors over 0.5 (where the quality factor varies between 0 – minimum, and 1 – maximum) [5]. In this work, our available extended CAPEC Lipids Database and CAPEC Lipids Mixtures Database is used for revising the Original UNIFAC model group contribution parameters for lipids by proposing new values, aimed to offer a better prediction of phase equilibria calculation (vapour-liquid equilibrium VLE, solid-liquid equilibrium, SLE). The regression of the new parameters is done using carefully selected VLE data sets, screened out for possible erroneous data. VLE data selection is performed based on the quality factor given by the different consistency tests available in ThermoData Engine (TDE) from NIST. More than 60 VLE data sets consisting of over 600 data points, available in CAPEC LIPIDS Mixture Database, are used for the regression of the 54 binary interaction parameters corresponding to 10 groups for Original UNIFAC model. Note that only 10 groups are needed to represent all the lipids data sets. However, to allow a better performance of the model for this type of systems, two new groups were introduced: one group is describing the behaviour of hydroxyl within mono and diglycerides (OHacyl) and another one is describing the glycerol molecule (GLY). The parameters are tested and evaluated on VLE and SLE data and by using a cross validation method. Compared to original UNIFAC, the performance of the new parameters for the lipids systems present a substantial improvement in
Phase Equilibrium Measurements and Modeling of 1-Propanethiol+1-Butanethiol + CH₄ in Methane Ternary System at 303, 336, and 368 K and Pressure Up to 9 MPa

New vapor-liquid equilibrium (VLE) data for 1-propanethiol + 1-butanethiol + CH₄ ternary system is reported. Measurements were performed at three different temperatures (303, 336, and 368 K), and the pressure ranged from 1 to 9 MPa. The total system pressure was maintained by CH₄. The inlet mole fraction of 1-propanethiol (x = 5.43 x 10⁻¹) and 1-butanethiol (x = 4.56 x 10⁻¹) in the liquid phase were same in all experiments. A static analytic method was used for performing phase equilibrium measurements. The new VLE data have been modeled successfully with cubic-plus-association (CPA) equation of state.
Phase equilibrium of North Sea oils with polar chemicals: Experiments and CPA modeling

This work consists of a combined experimental and modeling study for oil - MEG - water systems, of relevance to petroleum applications. We present new experimental liquid-liquid equilibrium data for the mutual solubility of two North Sea oils + MEG and North Sea oils + MEG + water systems in the temperature range 303.15-323.15 K and at atmospheric pressure. These new data are for North Sea oils which are substantially heavier and with higher aromatic/naphthenic content compared to previous studies. The new data compare favorably with previously reported measurements for other North Sea oils. The data have been successfully modeled using the Cubic-Plus-Association (CPA) equation of state (EoS) using a previously developed characterization method and new correlations for estimating binary interaction parameters between MEG-hydrocarbons and water-hydrocarbons. The results are in satisfactory agreement to the experimental data, considering especially the complexity of the studied reservoir fluids, in particular their heavy and aromatic character.

General information

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Phenomena Based Process Intensification of Toluene Methylation for Sustainable Para-xylene Production

The objective of this work is to generate more sustainable intensified process designs for the production of important chemicals in the petrochemical sector. A 3-stage approach is applied. In stage 1, the base case design is generated or selected from literature. In stage 2, the base case design is analysed in terms of economics, sustainability and LCA factors in order to identify process hot-spots that are translated into design targets. In stage 3, intensified flowsheet alternatives are generated that match the targets and thereby eliminate and/or minimize the process hot-spots using a phenomena based method. Here, the flowsheet is decomposed into unit operations, tasks and phenomena that are analysed and selected in order to increase driving forces related to, for example, reaction and separation. The phenomena are then recombined to fulfill tasks that are translated into intensified unit operations to generate more sustainable designs. An overview of the key concepts and framework are presented together with the results from a case study highlighting the application of the framework to the sustainable design of a production process for para-xylene, which is an important chemical utilized in the production of polymers such as polyesters.

Physical Properties for Lipids Based Process and Product Design

Lipid processing covers several oil and fats technologies such as: edible oil production, biodiesel production, oleochemicals (e.g.: food additives, detergents) and pharmaceutical product manufacturing. New demands regarding design and development of better products and more sustainable processes related to lipids technology, emerge according to consumers demanding improved product manufacturing from sustainable resources and new legislation regarding environmental safety [1]. Physical and thermodynamic property data and models for prediction of pure compound properties and mixtures properties involving lipids represent the basic and most important requirements for process product design, simulation and optimization. Experimentally measured values of involved compounds are desirable, but in most of the cases these are not available for all the compounds and properties needed. The lack of properties is even larger for mixtures properties. Therefore there is a highly need of predictive properties models.

General information
Phytase application in chewing gum - A technical assessment

Phytase catalysis has been shown to improve iron absorption by dephosphorylation of the potent iron chelator, phytic acid, found in high amounts in cereals. Recently, the World Health Organization evaluated the phytase from Aspergillus niger as safe for use in human food. The phytase may work either prior to ingestion, i.e. in the food, or post ingestion, i.e. in the human gastrointestinal tract. We have assessed the technical aspects of formulation and release of phytase added to chewing gum as a delivery vehicle. Phytases from Aspergillus niger and Escherichia coli incorporated into chewing gum were released quantitatively upon chewing and retained phytase activity (50-80% of the enzyme activity added was released within 10 minutes). Initial evaluations of phytase chewing gum shelf life showed good stability after 48 days of storage of the chewing gum at ambient conditions.

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Phytase-mediated mineral solubilization from cereals under in vitro gastric conditions: Phytase-mediated mineral release

BACKGROUND
Enzymatic dephosphorylation of phytic acid (inositol hexakisphosphate) in cereals may improve mineral bioavailability in humans. This study quantified enzymatic dephosphorylation of phytic acid by measuring inositol tri- to hexakisphosphate (InsP3-6) degradation and iron and zinc release during microbial phytase action on wheat bran, rice bran and sorghum under simulated gastric conditions.

RESULTS
InsP3-6 was depleted within 15–30 min of incubation using an Aspergillus niger phytase or Escherichia coli phytase under simulated gastric conditions with the two enzymes dephosphorylating cereal phytic acid at similar rates and to similar extents. Microbial phytase-catalysed phytate dephosphorylation was accompanied by increased iron and zinc release from the cereal substrates. For wheat bran at pH 5, the endogenous wheat phytase activity produced mineral release equal to or better than that of the microbial phytases. No increases in soluble cadmium, lead or arsenic were observed with microbial phytase-catalyzed phytate dephosphorylation.

CONCLUSION
Microbial phytase treatment abated phytate chelation hence enhanced the release of iron and zinc from the phytate-rich cereals at the simulated gastric conditions. The data infer that acid stable microbial phytases can help improve iron bioavailability from phytate-rich cereal substrates via post-ingestion activity.
Phytases for improved iron absorption

Phytase enzymes present an alternative to iron supplements, because they have been shown to improve iron absorption by means of catalysing the degradation of a potent iron absorption inhibitor: phytic acid. Phytic acid is a hexaphosphate of inositol and is particularly prevalent in cereal grains, where it serves as a storage molecule for phosphorous. Phytic acid is also associated with minerals. The minerals are bound by chelation to the negatively charged phosphate groups in phytic acid. Phytases catalyse the dephosphorylation of phytic acid, thus releasing bound minerals to make them available for absorption. This article presents research on phytase catalysis in gastric conditions and considers potential benefits and
drawbacks for using phytases as a food supplement.
Pitfalls of using the geometric-mean combining rule in the density gradient theory

It is popular and attractive to model the interfacial tension using the density gradient theory with the geometric-mean combining rule, in which the same equation of state is used for the interface and bulk phases. The computational efficiency is the most important advantage of this theory. In this work, it has been mathematically shown that the theory fails if the solution profile is not monotonic in the path function, which is defined as the summation of the density multiplied by the square root of the influence parameter over all components. A computational solution procedure is then presented by specifying the path function, in which a reference component is not needed. The differences of the chemical potential between the interface and the bulk phases, and the tangent plane distance have been used to analyze the characteristics of the solution profile from the geometric-mean density gradient theory. It has been found that the solution profile passes a saddle point of the tangent plane distance, which is independent of the influence parameters. It has been shown that the numerical pitfalls could occur for both vapor liquid and liquid liquid equilibrium systems. Shape density change inside the interface could be considered as a warning for the unsuccessful applications of the geometric-mean density gradient theory combined with the chosen thermodynamic model, even if numerical pitfalls do not occur. (C) 2016 Elsevier B.V. All rights reserved.
Plant growth responses to elevated atmospheric CO₂ are increased by phosphorus sufficiency but not by arbuscular mycorrhizas

Capturing the full growth potential in crops under future elevated CO₂ (eCO₂) concentrations would be facilitated by improved understanding of eCO₂ effects on uptake and use of mineral nutrients. This study investigates interactions of eCO₂, soil phosphorus (P), and arbuscular mycorrhizal (AM) symbiosis in Medicago truncatula and Brachypodium distachyon grown under the same conditions. The focus was on eCO₂ effects on vegetative growth, efficiency in acquisition and use of P, and expression of phosphate transporter (PT) genes. Growth responses to eCO₂ were positive at P sufficiency, but under low-P conditions they ranged from non-significant in M. truncatula to highly significant in B. distachyon. Growth of M. truncatula was increased by AM at low P conditions at both CO₂ levels and eCO₂×AM interactions were sparse. Elevated CO₂ had small effects on P acquisition, but enhanced conversion of tissue P into biomass. Expression of PT genes was influenced by eCO₂, but effects were inconsistent across genes and species. The ability of eCO₂ to partly mitigate P limitation-induced growth reductions in B. distachyon was associated with enhanced P use efficiency, and requirements for P fertilizers may not increase in such species in future CO₂-rich climates.

General information
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Plant-wide modelling and control of nitrous oxide emissions from wastewater treatment plants

Nitrous oxide ($N_2O$) is a greenhouse gas with a global warming potential three hundred times stronger than carbon dioxide (CO2). The IPCC report released in 2014 shows that the CO2 equivalents emitted from the wastewater systems are increasing in the last decades. It was also estimated that 14% of those CO2 equivalents comes from $N_2O$ emissions. It becomes therefore relevant, within the context of reducing the carbon footprint of wastewater treatment (WWT) systems, to develop control strategies aimed at the minimization of the emissions of this gas. Till now, few operation strategies have been developed to reduce the amount of $N_2O$ emitted from WWTP plants. However, these strategies have been employed for mainly sequencing-batch systems, where mere regulations of the cycle frequency and/or of the length of aeration and anoxic phases are enough to drastically reduce the amount of $N_2O$ emissions. However, in full-scale continuously-aerated wastewater treatment systems such control strategies cannot be implemented. Furthermore, the available control strategies developed for $N_2O$ emissions are not online, namely they do not change the operating conditions automatically as a function of on-line measurements. All of this makes the technologies proposed till now too case-specific and quite a number of adaptations would be needed if the system is changed. During the present work, a generic control strategy for $N_2O$ emission minimization is developed. More specifically, the control strategy is designed in order to prevent the typical biologial mechanisms triggering $N_2O$ production. Furthermore, for thorough and comprehensive evaluation of such a control strategy prior to its application in real full-scale WWT systems, the developed control strategy is implemented and simulated in different model environments and a multi-criteria evaluation, taking into account not only the $N_2O$ emissions but also the effluent quality and the operational costs, is carried out. This is because the reduction of the carbon footprint of WWTP plants cannot be achieved at the expense of worse effluent quality and unreasonably-high operational costs. To build simulation environments where $N_2O$ controller could be benchmarked against a reference scenario, three different benchmark simulation models are developed by including $N_2O$-producing processes in the Benchmark Simulation Model No2. As an outcome, three different benchmark simulation models - the BSM2Na, the BSM2Nb and the BSM2Nc – are available. A scenario analysis showed discrepancies among the $N_2O$ predictions by the three models. Since there is at the moment no consensus model considered to describe reliably $N_2O$ emissions from WWTP plants, all the three models are used for testing the $N_2O$ control strategy. In a second step, a comprehensive sensitivity analysis on the BSM2Na was carried out at the aim of extrapolating the main biological mechanisms responsible for $N_2O$ emissions. It was found that the ratio between NOB and AOB activity could indicate the accumulation of those nitrification intermediates, like nitrite and hydroxylamine, which trigger the $N_2O$ production via AOB denitrification. Given the interactive nature and multiple objectives typically required in biological systems, fuzzy-logic approach was chosen as a control technique for the implementation of the strategy. To avoid poor performance behaviour due to intuitive design, a systematic procedure for the design of fuzzy-logic controllers is developed using a partial nitritation/Anammox system as application case. The same systematic methodology is then adopted to tune the fuzzy-logic controller for low $N_2O$ emissions. The ratio between measured nitrate produced and ammonium consumed in the aerobic zone (RNatAmm) is used as controlled variable and oxygen supply is regulated accordingly. The results coming from the benchmarking of the control strategy in the three simulation models showed that, by controlling the ratio RNatAmm, $N_2O$ emissions were able to be drastically reduced within reasonable aeration energy consumptions. To cope with the increased COD demand by heterotrophic denitrifiers, additional control actions regulating the flow rate for carbon addition in the anoxic compartment were implemented. The results of the controller evaluated under comprehensive simulation tests indicate a promising potential for full-scale applications in order to reduce $N_2O$ emission from WWTPs. In addition, implementation of the control concept requires minimum investment (only relevant sensors required and adaptation of aeration control algorithm of the plants) is expected to encourage its take up by WWT plant operators for managing CO2 footprints of WWTPs.
Poisoning of vanadia based SCR catalysts by potassium: influence of catalyst composition and potassium mobility

The deactivation of V$_2$O$_5$–(WO$_3$)/TiO$_2$ catalysts for selective catalytic reduction (SCR) of NO$_x$ upon exposure to aerosols of KCl or K$_2$SO$_4$, at different temperatures, has been studied. All samples exposed for more than 240 hours lost a substantial fraction of their initial activity although lower exposure temperatures slowdown the deactivation. K$_2$SO$_4$ causes a lower rate of deactivation compared to KCl. This may be related to a faster transfer of potassium from the solid KCl matrix to the catalyst, however, it cannot be ruled out also be caused by a significantly larger particle size of the K$_2$SO$_4$ aerosol (mass based distribution mode: 1.3 μm) compared to that of the KCl aerosol (mass based distribution mode: 0.12 μm). The relative activities of exposed catalysts indicate that promotion with WO$_3$ accelerates the deactivation, likely due to the enhanced Brønsted acidity which appears to promote the transport of potassium. Using a newly developed experimental protocol consisting of two-layer pellets of SCR catalysts, where one side is impregnated with KCl or K$_2$SO$_4$, the potassium transport in such systems, which is assumed to take place through reaction and diffusion over acid sites, was investigated. SEM-WDS measurements on pellets heat treated at 350 °C showed that potassium bound in KCl readily leaves its counter ion and thus moves faster into the catalyst compared to potassium from K$_2$SO$_4$, which is in agreement with results from the aerosol exposures.
Polyhydroxyalkanoates (PHA) production from fermented crude glycerol by mixed microbial cultures.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, PILOT PLANT, The Danish Polymer Centre
Authors: Burniol Figols, A. (Intern), Varrone, C. (Intern), Daugaard, A. E. (Intern), Skiadas, I. V. (Intern), Gavala, H. N. (Intern)
Number of pages: 1
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Pore-size distribution and compressibility of coarse sandy subsoil with added biochar

Sustainable agricultural production on coarse sandy soil is constrained by the restricted growth of roots, and poor water and nutrient retention. Amending the soil with biochar can reduce these problems, but the processes involved are not known in detail. We investigated in the laboratory the effects of two fine-grained gasification biochars made of straw (LTST) and other materials (LTSN) and of one fast pyrolysis straw biochar (FPST) on pore-size distribution and soil compressibility when added to coarse sandy subsoil. Water retention and therefore pore-size distribution were affected systematically. All biochars converted drainable pore space with pore diameters in the range 60–300 µm into water-retaining pores of size 0.2–60 µm, which was taken as an estimate of available water capacity (AWC). Effects were linear over the whole range of biochar (0–4% by mass). The effect of LTST and LTSN on AWC (3.6% by volume per % biochar) was about 70% larger than the effect of the somewhat coarser FPST biochar (2.1% by volume per % biochar). The compression index increased linearly with biochar content without any significant effects from the type of biochar. The common least squares estimate of the slope was 21.2 kg m⁻³ %⁻¹ by weight. The results reflect a strong interaction at the microscopic scale between biochar and soil rather than intrinsic properties of the added biochar.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Copenhagen, Roskilde University
Authors: Petersen, C. T. (Ekstern), Hansen, E. (Ekstern), Larsen, H. H. (Ekstern), Hansen, L. V. (Ekstern), Ahrenfeldt, J. (Intern), Hauggaard-Nielsen, H. (Ekstern)
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Potential challenges of biogas from fish industry waste in the Arctic

The fish industry is a main industry in many Arctic locations. In most places by-products are disposed of at sea. Oxygen depletion and dead sea bottom is observed, as the organic material is biodegraded and methane produced; contributing to the global warming. In this study, the biogas potential of fish industry by-products from Greenland was investigated. Methane potential of Greenlandic shrimp, crab, and halibut by-products as well as co-digestion of shrimp by-products with waste water sludge and common brown algae was tested in lab scale batch experiments at mesophilic conditions. Fate of indicator microorganisms was investigated. All residues had biogas potentials similar to or higher than conventional feedstocks like manure and silage. Waste water sludge and brown algae had potentials comparable to manure. The combined shrimp and algae digestion showed indication of synergistic effects. Indicator bacteria were reduced significantly while coliphages (virus indicators) were not. Fish and seafood by products from the fish processing industry constitute a significant resource for energy and may provide an economic incentive to install digesters, which can also partly stabilize waste water sludge, though additional heat treatment may be necessary depending on final use of digestate.

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Organisations: Department of Civil Engineering, ARTEK, Section for Arctic Engineering and Sustainable Solutions, Department of Chemical and Biochemical Engineering
Authors: Jensen, P. E. (Intern), Heiske, S. (Intern)
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Prediction and experimental determination of the solubility of exotic scales at high temperatures - Zinc sulfide

The presence of "exotic" scale such as Zinc Sulfide (ZnS), Lead Sulfide (PbS) and Iron Sulfide (FeS) in HP/HT reservoirs has been identified. "Exotic" scale materials come as a new challenge in HP/HT reservoirs. This has led to the development of more advanced tools to predict their behavior at extreme conditions. The aim of this work is to include ZnS into the group of scale materials that can be modeled with the Extended UNIQUAC model. Solubility data for ZnS are scarce in the open literature. In order to improve the available data, we study the experimental behavior of ZnS solubility at high temperatures. The determination of the solubility of ZnS is carried out at temperatures up to 250°C. Zinc sulfide (99.99%) and ultra-pure water are placed in a vial in a reduced oxygen atmosphere. The sample is placed in a controlled bath and stirred until equilibrium is attained. The suspension is filtered at the same process temperature and diluted immediately. Afterwards the aqueous solution is analyzed using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) as analytical technique. The concentrations of Zn²⁺ and S²⁻ ions are analyzed. The experimental data are used for parameter estimation in the Extended UNIQUAC model presented by Villafafila et al. (2005); (2006). The solid-liquid phase equilibria of the system is represented using the Extended UNIQUAC model. This model is chosen due to its versatility and fewer number of parameters (two parameters per species plus two parameters per species pair) to be estimated compared to other models (Pitzer's model). It is observed that ZnS solubility increases with increasing the temperature. This temperature dependency is very well represented by the Extended UNIQUAC model. The model is capable of predicting experimental data within the experimental error. The agreement between experimental data and the Extended UNIQUAC model shows that this thermodynamic model is a promising tool capable of determining the occurrence of ZnS scaling in HP/HT reservoirs. This methodology can be extended to other scaling materials (PbS, FeS), making the Extended UNIQUAC model a leading model in predicting scaling in HP/HT reservoirs.
Predictive Modelling of Phase-Transfer Catalyst Systems for Improved and Innovative Design

Phase-transfer catalyst (PTC) systems contain two immiscible liquid phases with a heterogeneous PTC transferring active ion from one phase to the other for converting the reactant to the desired product, and in the process generating the inactive ion. This type of reacting systems is receiving increasing attention as a novel organic synthesis option due to its flexible and easier operation, higher production yield, and ability to eliminate expensive solvents, although, not eliminating the use of solvents.

New mathematical models of the PTC system, which includes physical and chemical equilibrium, reaction mechanism and unit operation has been developed. In the developed model, the PTC system is divided into four sub-systems of aqueous-organic solvent partition, inorganic salt in aqueous phase, PTC in aqueous phase, and PTC in aqueous phase. Each subsystem requires an appropriate thermodynamic model to predict the partition and equilibrium of the involved species. A new predictive electrolyte model (e-KT-UNIFAC) that has the capability to predict the partition and equilibrium of systems containing novel PTCs has been embedded into the reactor model. With this option, the application range has been significantly widened, making it feasible to identify new and innovative biphasic reaction options.

In this paper, the predictive qualities of the new model together with the improvements in the predicted design and operation of reaction with PTC systems are highlighted. Also, applications of problem-specific models for selecting improved design alternatives based on different design targets are presented.
Predictive screening of ionic liquids for dissolving cellulose and experimental verification

In this work, 357 ionic liquids (ILs) formed from 17 cations and 21 anions were selected for evaluation of their ability to dissolve cellulose by COSMO-RS. In order to evaluate the predictive model and method, experimental measurements of the solubility of microcrystalline cellulose (MCC) in 7 of these ILs were also conducted. Predicted results from logarithmic activity coefficients were generally in good agreement with the experimental results. Three different models were used for describing cellulose, and the mid-monomer part of the cellotriose model was found to be closer to the experimental results than a neat glucose model and the model of the mid-dimer part of celletetraose. Excess enthalpy calculations indicated that hydrogen-bond (H-bond) interactions between cellulose (i.e. the three cellulose models) and the 7 studied ILs are key factors for the solubility of cellulose, and the anions play a crucial role in the cellulose dissolution process. Importantly, the cations of methylimidazolium+, pyridinium+, ethylmorpholinium+ and methylpyrrolidinium+ structured with functional groups including ethyl, allyl, 2-hydroxyethyl, 2-methoxyethyl and acryloyloxypropyl, combined with anions Ac−, Dec−, HCOO−, Cl−, BEN−, DMPO4−, DEP−, DBP− and Br− were predicted to be the best for dissolving cellulose.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, CERE – Center for Energy Ressources Engineering, Chinese Academy of Sciences
Authors: Liu, Y. (Intern), Thomsen, K. (Intern), Nie, Y. (Ekstern), Zhang, S. (Ekstern), Meyer, A. S. (Intern)
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Scopus rating (2013): SJR 2.266 SNIP 1.815 CiteScore 7.44
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Scopus rating (2012): SJR 2.439 SNIP 1.709 CiteScore 6.64
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Scopus rating (2011): SJR 2.363 SNIP 1.697 CiteScore 6.46
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Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.152 SNIP 1.655
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Scopus rating (2009): SJR 2.101 SNIP 1.791
BFI (2008): BFI-level 2
Preface
This special issue of Computers & Chemical Engineering contains extended versions of selected papers from the joint event of the 12th International Symposium on Process Systems Engineering (PSE) and the 25th European Symposium on Computer Aided Process Engineering (ESCAPE) held in Copenhagen during 31 May to 4 June 2015. These papers were recommended by the International Programming Committee and constitute a representative sample of the invited plenary lectures, invited keynote lectures, and contributed papers.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Huusom, J. K. (Intern), Gani, R. (Intern)
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Preface: Catalysis Today: Special issue of Catalysis Today with the theme “Sustainable Energy”
This special issue of Catalysis Today with the theme “Sustainable Energy” results from a great success of the session “Catalytic Technologies Accelerating the Establishment of Sustainable and Clean Energy”, one of the two sessions of the 1st International Symposium on Catalytic Science and Technology in Sustainable Energy and Environment, held in Tianjin, China during October 8–10, 2014. This biennial symposium offers an international forum for discussing and sharing the cutting-edge researches and the most recent breakthroughs in energy and environmental technologies based on catalysis principles. A total of 29 invited contributions from the authors who made oral and poster (very limited number) presentations are included in this special issue. A wide spectrum of topics is covered, which can be broadly categorized as:
- Clean Fossil Fuels
- Renewable Fuels
- Efficient Catalytic Energy Processors
Finally, we gratefully acknowledge all the authors and reviewers of the manuscripts and the editorial team of Elsevier, without whom the special issue would not have been possible.

General information
Preparation and characterization of MgB2 with Pd, Pt and Re doping

Samples with Mg1-xDxB2.04 (D = Pt, Pd or Re) nominal compositions have been synthesised by a solid-state route. None of these doping elements can be substituted for Mg in a detectable amount and their presence in the samples has no influence on the critical temperature and on the lattice parameters of the MgB2 superconductor. Impurity phases are formed by reaction mostly with Mg. The microstructure of the Pt, Pd and Re-based phases depends on the elements. Re-rich particles with large sizes up to 8 μm form, whereas Pt- and Pd-containing impurities are finely dispersed with a particle size that does not exceed 1 μm. The field dependence of the normalised critical current density is improved when Pt, Pd or Re are present in the samples.
Pretreatment of hemp fibers for utilization in strong biocomposite materials

Hemp is the common name for Cannabis sativa cultivated for industrial use. Compared to synthetic fibers (e.g. glass fiber), hemp fibers have many advantages such as low cost, low density (1.5 g/cm³) and high specific strength and stiffness. As a result of increasing environmental awareness, interest in hemp fiber reinforced composites is increasing because of its high potential of manufacturing hemp fiber reinforced polymer composites with acceptable mechanical properties at low cost. In order to expedite the application of natural fibers in polymer composites, hemp fibers need to be treated before being incorporated in matrix polymers to optimize the properties of fibers and fiber reinforced composites. The overall objective of this study was therefore to focus on understanding the correlation between chemical composition and morphology of hemp fibers and mechanical properties of hemp fibers, and furthermore to establish the relationship between the mechanical properties of hemp fiber reinforced composites and the chemical composition and morphology of hemp fibers after different fiber treatments.

The first part of this study investigated the effect of harvest time and stem sections on mechanical properties of hemp fibers in order to correlate the mechanical properties of hemp fibers to their chemical composition and morphology. Harvest time (or growth stage) and stem sections were found to have an effect on the mechanical properties of hemp fibers. The variations in mechanical properties of hemp fibers can be explained by the differences in chemical composition and morphology. Untreated hemp bastfibers with high cellulose content had high stiffness and tensile strength. In addition, the presence of secondary fibers was found to reduce the favorable mechanical properties of hemp fibers. It was our intention to find the key factors that damage fiber properties during traditional field retting. In order to compare and
Probe the Binding Mode of Aristololactam-β-D-glucoside to Phenylalanine Transfer RNA in Silico

Understanding the interactions of drug molecules with biomacromolecules at a micro-scale level is essential to design potent drugs for the treatments of human genome diseases. To unravel the mechanism of binding of aristololactam-β-D-glucoside (ADG) and phenylalanine transfer RNA (tRNA\textsuperscript{Phe}), an integrated computational strategy combining quantum mechanics (QM) calculation, molecular docking and atomistic molecular dynamics (MD) simulation was present in this work. QM calculations were performed to derive the partial charges of ADG, molecular docking was used to determine the binding poses of ADG on the tRNA\textsuperscript{Phe}, and atomistic MD simulations were conducted to examine the thermal stability of five predicted binding poses for the complex of ADG and the tRNA\textsuperscript{Phe}. The binding free energies of the five complexes were then calculated using the molecular mechanics/generalized born surface area approach with the variable internal dielectric constant model. By comparing computed affinities and experimentally-measured values in the binding free energy model, by comparing computed affinities and experimentally-measured values in the binding free energy...
energy, we identified a most likely binding structure of ADG and the tRNAPhe. Further analysis of energy of the ADG-tRNA complex revealed that the aristololactam of ADG provides binding specificity to the tRNAPhe, and the D-glucose contributes to the affinity for binding with the tRNAPhe.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, North Carolina State University, Wuhan Institute of Technology, East China University of Science and Technology
Authors: Xiao, X. (Ekstern), Zhao, B. (Ekstern), Yang, L. (Ekstern), Liang, X. (Intern), Ren, Y. (Ekstern)
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**Process Evaluation Tools for Enzymatic Cascades Welcome Message**

Biocatalysis is attracting significant attention from both academic and industrial scientists due to the excellent capability of enzyme to catalyse selective reactions. Recently, much interest has been shown in the application of enzymatic cascades as a useful tool in organic synthesis to synthesize valuable compounds (e.g. chiral molecules) especially as pharmaceutical intermediates and to assist complex reactions that otherwise has problems as single step system. Despite this interest, process evaluation of many enzymatic cascades has only rarely been reported in the search for process improvement and implementation. Hence, the goal of this thesis is to evaluate the process concepts in enzymatic cascades in a systematic manner, using tools such as thermodynamic and kinetic analysis. Three relevant case studies have been used to exemplify the approach.

In the first case study, thermodynamic and kinetic studies were used to evaluate the favourability of a redox neutral cascade for the asymmetric amination of alcohols to their corresponding chiral amines. This synthetic cascade is potentially attractive since it synthesizes valuable chiral molecule from cheap raw materials as well as maximising the atom economy. The scheme consists of two primary enzymes (alcohol dehydrogenase and ω-transaminase) that are directly involved in the main synthesis. Alanine dehydrogenase was introduced as a secondary enzyme to regenerate the co-factor NAD⁺ and co-substrate alanine in situ as well as to shift the equilibrium positions in the main syntheses. In principle, this strategy could successfully achieve high conversion, using ammonia as the sole reagent used in excess to drive the conversion. The findings herein indicate that quantitatively the possibilities for improving the conversion of thermodynamically limited reactions are not only via application of enzyme coupling reactions (coupling the unfavourable reaction with an energetically favourable reaction) but also by matching the relative reaction rates between the interconnecting enzymes.

When the reaction steps are independent in a cascade, the kinetics can be controlled in a highly efficient way to achieve a sufficiently favourable conversion to a given target product. This is exemplified in the second case study, in the kinetic modelling of the formation of 2-ketoglutarate from glucoronate, the second case study. This cascade consists of 4 enzymes (uronate dehydrogenase, glucarate dehydratase, keto-deoxy-d-galactarate dehydratase and α-ketoglutaric semialdehyde dehydrogenase) run in that order to successfully achieve high conversion.

Finally, a third case study was used to explore the effect of activity-coefficients in enzyme-catalysed reactions. Frequently, the 'apparent' or (concentration-based) equilibrium constant (K'), instead of activity-based equilibrium constant, was used to describe reaction equilibria of biological systems. It is assumed that the reactant activity is equal to the respective reactant molar concentration at equilibrium since many reactions operate in dilute aqueous solutions and thus neglect the activity coefficient effect. The effect of such assumption was therefore tested with the cyclohexanone amination with (S)-1-phenylethylamine catalysed by ω-transaminase. The findings showed that the activity coefficients of the components significantly deviate from unity, indicating its non-ideal behaviour in the reaction medium.

Hence, thermodynamic and kinetic analyses are powerful tools to evaluate and to achieve workable cascades for non-
natural pathways. Additionally, more meaningful equilibrium data from enzyme-catalysed reactions can be a useful way to determine the effectiveness of a given cascade strategy.

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**Relations**
Projects:

**Process limitations of a whole-cell P450 catalyzed reaction using a CYP153A-CPR fusion construct expressed in Escherichia coli**
Cytochrome P450s are interesting biocatalysts due to their ability to hydroxylate non-activated hydrocarbons in a selective manner. However, to date only a few P450-catalyzed processes have been implemented in industry due to the difficulty of developing economically feasible processes. In this study, we have used the CYP153A heme domain from Marinobacter aquaefaciatus fused to the reductase domain of CYP102A1 from Bacillus megaterium (BM3) expressed in Escherichia coli. This self-sufficient protein chimera CYP153A-CPRBM3 G307A mutant is able to selectively hydroxylate medium and long chain length fatty acids at the terminal position. ω-Hydroxylated fatty acids can be used in the field of high-end polymers and in the cosmetic and fragrance industry. Here, we have identified the limitations for implementation of a whole-cell P450-catalyzed reaction by characterizing the chosen biocatalyst as well as the reaction system. Despite a well-studied whole-cell P450 catalyst, low activity and poor stability of the artificial fusion construct are the main identified limitations to reach sufficient biocatalyst yield (mass of product/mass of biocatalyst) and space-time yield (volumetric productivity) essential for an economically feasible process. Substrate and product inhibition are also challenges that need to be addressed, and the application of solid substrate is shown to be a promising option to improve the process.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Stuttgart, University of Natural Resources and Life Sciences
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Web of Science (2017): Indexed yes
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This paper reviews issues and applications for design of sustainable carbon dioxide conversion processes, specifically through chemical conversion, and the integration of the conversion processes with other systems from a process systems engineering (PSE) viewpoint. Systematic and computer-aided methods and tools for reaction network generation, processing route generation, process design/optimization, and sustainability analysis are reviewed with respect to carbon dioxide emissions through conversion technologies.
dioxide conversion. Also, the relevant gaps and opportunities are highlighted. In addition, the integration of carbon dioxide conversion processes with other systems including coexisting infrastructure and carbon dioxide sources is described. Then, the importance of PSE based studies for such application is discussed. Finally, some perspectives on the status and future directions of carbon dioxide conversion technology and the development and use of PSE approaches are given.

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, Korea Advanced Institute of Science & Technology
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Web of Science (2016): Indexed yes
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
Web of Science (2014): Indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.912 SNIP 1.335 CiteScore 2.12
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.87 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.742 SNIP 1.029
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.645 SNIP 0.718
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.572 SNIP 0.787
Scopus rating (2006): SJR 0.629 SNIP 0.823
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.752 SNIP 1.02
Productivity and carbon footprint of perennial grass-forage legume intercropping strategies with high or low nitrogen fertilizer input

A three-season field experiment was established and repeated twice with spring barley used as cover crop for different perennial grass-legume intercrops followed by a full year pasture cropping and winter wheat after sward incorporation. Two fertilization regimes were applied with plots fertilized with either a high or a low rate of mineral nitrogen (N) fertilizer. Life cycle assessment (LCA) was used to evaluate the carbon footprint (global warming potential) of the grassland management including measured nitrous oxide (N2O) emissions after sward incorporation. Without applying any mineral N fertilizer, the forage legume pure stand, especially red clover, was able to produce about 15 t aboveground dry matter ha⁻¹ year⁻¹ saving around 325 kg mineral N fertilizer ha⁻¹ compared to the cocksfoot and tall fescue grass treatments. The pure stand ryegrass yielded around 3 t DM more than red clover in the high fertilizer treatment. Nitrous oxide emissions were highest in the treatments containing legumes. The LCA showed that the low input N systems had markedly lower carbon footprint values than crops from the high N input system with the pure stand legumes without N fertilization having the lowest carbon footprint. Thus, a reduction in N fertilizer application rates in the low input systems offsets increased N2O emissions after forage legume treatments compared to grass plots due to the N fertilizer production-related emissions. When including the subsequent wheat yield in the total aboveground production across the three-season rotation, the pure stand red clover without N application and pure stand ryegrass treatments with the highest N input equalled. The present study illustrate how leguminous biological nitrogen fixation (BNF) represents an important low impact renewable N source without reducing crop yields and thereby farmers earnings.
Computer-aided molecular design (CAMD) helps in the reduction of experiments for the selection/design of optimal working fluids. In reducing the number of experiments, solutions obtained by trial and error is replaced by solutions that are based on mixture-process properties.
In generating optimal working fluid candidates a database is required that can be simultaneously searched in order to differentiate and determine whether the generated candidates are existing or novel. Also, the next step upon selection of the candidates is performing experiments in order to test and verify the generated working fluids. If performed properly, the experimental step is solely verification. Experiments can either be performed virtually (in order to further reduce the number of required experiments) and/or physically. Therefore the objective of this work was the development of a database of existing working fluids and their properties and the development of a design of experiments method for verifying the optimal working fluids generated from CAMD

**Promoted V_{2}O_{5}/TiO_{2} catalysts for selective catalytic reduction of NO with NH_{3} at low temperatures**

The influence of varying the V_{2}O_{5} content (3–6 wt.%) was studied for the selective catalytic reduction (SCR) of nitrogen oxides by ammonia on heteropoly acid (HPA)- and tungsten oxide (WO_{3})-promoted V_{2}O_{5}/TiO_{2} catalysts. The SCR activity and alkali deactivation resistance of HPA-promoted V2O5/TiO2 catalysts was found to be much higher than for WO3-promoted catalysts. By increasing the vanadium content from 3 to 5 wt.% the catalysts displayed a two fold increase in activity at 225 °C and retained their initial activity after alkali doping at a molar K/V ratio of 0.181. Furthermore, the catalysts were characterized by N2 physisorption, XRPD, NH3-TPD, H2-TPR, Raman, FTIR and EPR spectroscopy to investigate the properties of the catalysts. XRPD, Raman and FTIR showed that promotion by 15 wt.% HPA does not cause V_{2}O_{5} to be present in crystalline form, also at a loading of 5 wt.% V_{2}O_{5}. Hence, use of HPAs does not cause increased N_{2}O formation or unselective oxidation of NH_{3}. Moreover, promotion by HPA instead of WO3 causes the catalysts to possess a higher number of acid sites, both in fresh and alkali poisoned form, which might explain their higher potassium tolerance. Ex-situ EPR spectroscopy revealed that HPA-promoted catalysts have higher V^{4+}/V^{3+} ratios than their WO3-promoted counterparts. H2-TPR suggests that HPAs do not have a beneficial effect on the V^{5+}/V^{3+} redox system, relative to WO3.
Propane Oxidation at High Pressure and Intermediate Temperatures

General information
State: Published
Property Model-based Tailor-made Design of Chemical-based Products

Computer-aided model-based methods and tools are increasingly playing important roles in chemical product design. They have the potential to very quickly search for and identify reliable product candidates that can then be verified through experiments. In this way, the time and resources spent on experiment are reduced leading to faster and cheaper to market the products. The tools also help to manage the solution of product design problems, which usually require efficient handling of model-data-knowledge from different sources and at different time and size scales.

The main contribution of this project is: (1) the development of a systematic model-based framework for chemical product design; (2) its implementation as a computer-aided tool based on a specially developed architecture; (3) the creation of product design template together with their algorithms, models, tools and data for various types of products. The goal has been to develop a chemical product simulator, similar in concept to a process simulator, which makes the product design and development easier and faster, and provide the way for unified and consistent product documentation. In the same way a typical process simulator works, the developed product simulator (VPPDLab) allows product designers to: (1) analyze chemicals based products by performing virtual experiments (product property and performance calculations); (2) predict the properties of products; and (3) create new product property and product performance models, when needed. However, unlike process simulators, VPPD-Lab can also be used directly for (4) design of chemicals based products using the design template for various types of products, such as, single molecule products, formulations, blends, emulsions and devices; and (5) create new product design templates when the needed template for a desired product is not available. VPPD-Lab employs a suite of algorithms such as database search, molecular and mixture blend design) and toolboxes such as property calculations and property model consistency tests for specific product property prediction, design, and/or analysis tasks.

In order to achieve the features mentioned above, several issues need to be addressed: the translation of consumer needs into target properties; property models and available data for each type of chemical products; design methods and algorithms; available computer-aided tools; the systematic framework for chemical product design and analysis and its implementation as architecture for VPPD-Lab. From many test problems, eight application examples are presented to illustrate the use of the software. For two of these examples, the prediction of product properties and the use of virtual experiments to test product performances are highlighted. Five examples illustrate the use of the product design templates with respect to five types of chemical products (molecular design, formulation design, emulsion design, blend design and device design).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, CERE – Center for Energy Resources Engineering
Authors: Kalakul, S. (Intern), Gani, R. (Intern), Kontogeorgis, G. (Intern)
Number of pages: 189
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Bibliographical note
PSE for SPEED Project

Relations
Projects:
Property Model-based Tailor-made Design of Chemical-based Products
Publication: Research › Ph.D. thesis – Annual report year: 2016
Protein-free cress seed gum (Lepidium sativum) was obtained by precipitation of crude cress seed gum (CSG) with ethanol followed by treatment with protease. Molecular weight, moisture, ash and uronic acids content decreased after elimination of protein. Elimination of protein improved significantly rheological proper-ties and thermal stability of cress seed gum. Mechanical spectra of the CSG and PFCSG were classified as weak gels and PFCSG showed stronger and more elastic network structure. The gum dispersions exhibited strong shear-thinning behavior which was described satisfactorily by the Herschel-Bulkley and Mooremodes. Protein-free cress seed gum had higher apparent and intrinsic viscosities than the crude gum. CSG indicated lower hysteresis loop area, but degree of structural recovery of the samples showed no significant difference. The main decomposition of PFCSG started above 213 \degree C with two peaks (at 261.72 \degree C and 306.58 \degree C) and initial decomposition temperature of CSG was 190.21 \degree C with one peak at 258.28 \degree C. DSC results coincided with those observed by thermogravimetric analysis. Enzyme treatment lowered the surface activity of CSG.
Purification of cress seed (*Lepidium sativum*) gum: Physicochemical characterization and functional properties

The aim of the present study was to investigate the effects of different purification methods (ethanol, isopropanol and ethanol-isopropanol) on the physicochemical and functional characteristics of cress seed gum. Sugar composition and molecular weight of the samples varied significantly. All the purification methods reduced ash and protein content and molecular weight of cress seed gum. The main decomposition of the purified samples started above 200º C and initial decomposition temperature of the crude gum was 190.21º C. DSC thermograms of the purified gums showed two exothermic events at 257.81-261.95 ºC and 302.46-311.57 ºC. Crude gum displayed an exothermic peak at 259.42º C. Sample I (purified using isopropanol) imparted the best surface activity among the purified samples as it had the highest protein and uronic acid contents and the lowest Mw. All the purification methods could improve emulsifying properties of cress seed gum and there was no significant difference among the purified samples. Crude gum showed the lowest foaming properties, while samples I and E (purified using ethanol) showed the highest foaming capacity and foam stability, respectively. (C) 2015 Elsevier Ltd. All rights reserved.

General information

State: Published
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.15 SJR 1.404 SNIP 1.745
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.46 SNIP 1.842 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
This article develops a methodology for quantifying the impact of flow maldistribution on the overall performance of a numbered-up microreactor system. The methodology consists of the simulation of multiple plug-flow microreactors in parallel where each microreactor is fed with a certain fraction of the total inlet flow. The modelling approach tests different flow maldistribution scenarios and quantifies their impact on the overall performance. This methodology can also be further used to study a configuration with N-microreactors in parallel, and to evaluate the sensitivity of the reaction under study.

The methodology is applied to two cases: 1) a test case, consisting of a first-order kinetic model, and 2) a case consisting of a conversion of benzylacetone and isopropylamine into 1-methyl-2-phenylpropylamine and acetone catalyzed by an aminotransferase. The methodology was found to be very flexible and could be used to identify potential bottlenecks and opportunities in the numbering-up approach.
Sialylated galactooligosaccharides (GOS) represent a potential infant formula ingredient, which is believed to contribute with a combination of the beneficial properties of the prebiotic GOS as well as of sialylated human milk oligosaccharides. Sialylated GOS do not exist in natural milk, but can be produced from κ(kappa)-casein glycomacropeptide (CGMP), a sialylated side stream component from cheese-making, by sialidase-catalyzed transsialylation. Using a rationally designed mutant of the sialidase from Trypanosoma rangeli, Tr13, with enhanced transsialylation activity, six different GOS preparations with a varying degree of polymerization (DP) were effectively sialylated with molar yields of 20-30% on the CGMP sialyl in batch reactions. The rate of sialylation of the individual DPs was largely dependent on the DP distribution in each GOS preparation, and Tr13 catalysis did not discriminate against large GOS molecules, providing the novelty point that GOS molecules are sialylated independently of their size by Tr13. Using CGMP, GOS, and Tr13, the production of gram-scale quantities of sialyl-GOS was achieved in 20L volume reactions. Compared to the benchmark transsialidase from pathogenic Trypanosoma cruzi, the Tr13 was significantly more thermostable. By employing an enzymatic membrane reactor, Tr13 could be recycled and after seven consecutive 1-h reaction cycles, the biocatalytic productivity of the enzyme was increased 7-fold compared to the batch reaction. Assuming that the enzyme may be specific for α-2,3-bound sialyl moieties only, and that only 50% of sialyl linkages in CGMP are α-2,3-linked, the molar yield of sialyl-GOS on the available α-2,3-bound sialyl moieties in CGMP reached 80% in the enzymatic membrane reactor system.
In this study, we introduce enzymatic perturbation combined with Fourier transform infrared (FTIR) spectroscopy as a concept for quantifying casein in subcritical heated skim milk using chemometric multiway analysis. Chymosin is a protease that cleaves specifically caseins. As a result of hydrolysis, all casein proteins clot to form a creamy precipitate, and whey proteins remain in the supernatant. We monitored the cheese-clotting reaction in real time using FTIR and analyzed the resulting evolution profiles to establish calibration models using parallel factor analysis and multiway partial least squares regression. Because we observed casein-specific kinetic changes, the retrieved models were independent of the chemical background matrix and were therefore robust against possible covariance effects. We tested the robustness of the models by spiking the milk solutions with whey, calcium, and cream. This method can be used at
different stages in the dairy production chain to ensure the quality of the delivered milk. In particular, the cheese-making industry can benefit from such methods to optimize production control.

**General information**

**State:** Published  
**Organisations:** Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, FOSS Analytical A/S, Arla Foods  
**Authors:** Baum, A. (Intern), Hansen, P. W. (Ekstern), Nørregaard, L. (Ekstern), Sørensen, J. (Ekstern), Mikkelsen, J. D. (Intern)  
**Pages:** 6071-9  
**Publication date:** 2016  
**Main Research Area:** Technical/natural sciences

**Publication information**

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**Volume:** 99  
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BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Web of Science (2017): Indexed Yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 2.66 SJR 1.304 SNIP 1.464  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 1.464 SNIP 1.498 CiteScore 2.63  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 1.43 SNIP 1.505 CiteScore 2.78  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 1.407 SNIP 1.597 CiteScore 2.82  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): SJR 1.451 SNIP 1.718 CiteScore 2.79  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 1.411 SNIP 1.59 CiteScore 2.59  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 1.351 SNIP 1.517  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 1.321 SNIP 1.717  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 1.226 SNIP 1.556  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 0.978 SNIP 1.894  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.169 SNIP 1.656  
Web of Science (2006): Indexed yes
Rational and Evolutionary Engineering of Industrial Saccharomyces Cerevisiae Strains for Production of Chemicals from Xylose-Rich Feedstocks

General information
State: Published
Organisations: Novo Nordisk Foundation Center for Biosustainability, Research Groups, Yeast Metabolic Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Stovicek, V. (Intern), Lis, A. V. (Intern), Borodina, I. (Intern), Förster, J. (Intern)
Number of pages: 1
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Publisher: American Institute of Chemical Engineers
Main Research Area: Technical/natural sciences
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Rational_and_Evolutionary_Engineering.pdf

Bibliographical note
Poster and rapid fire presentation
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Reaction invariant-based reduction of the activated sludge model ASM1 for batch applications
In any system, there are some properties, quantities or relationships that remain unchanged despite the applied transformations (system invariants). For a batch reaction system with n linearly independent reactions and m components (n<m) there exist linear combinations of the concentrations that are unaffected by the reaction progress, i.e. so-called reaction invariants. The reaction invariant concept can be used to reduce the number of ordinary differential equations (ODEs) involved in batch bioreactor models. In this paper, a systematic methodology of model reduction based on this concept is applied to batch activated sludge processes described by the Activated Sludge Model No. 1 (ASM1) for carbon and nitrogen removal. The objective of the model reduction is to describe the exact dynamics of the states predicted by the original model with a lower number of ODEs. This leads to a reduction of the numerical complexity as nonlinear ODEs are replaced by linear algebraic relationships predicting the exact dynamics of the original model.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Tecnologica Nacional Facultad Regional Rosario
Authors: Santa Cruz, J. A. (Ekstern), Mussati, S. F. (Ekstern), Scenna, N. J. (Ekstern), Gernaey, K. (Intern), Mussati, M. C. (Ekstern)
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Publication date: 2016
Remotely Activated Microcapsules for Oil Recovery Treatments

Water-flooding is a commonly used oil recovery method in mature reservoirs, because injected water enhances oil sweep efficiency and leads to increased oil production. Due to the occurrence of fractures in water-flooded reservoirs, excessive water production is observed. Hence, water shut-off treatments are extensively investigated, though currently applied materials still suffer from some disadvantages. The main drawback is lack of control over the setting of plugs in the fracture, and this may cause blocking of the injection well and the formation of the plug before placing the material in the fracture. Secondly, only a few developed materials prevent from blocking oil-rich pores, and yet they are not able to create a permanent plug, as they do not form a covalently bonded structure.

The aim of the project is to design a novel plugging material which can block fractures without affecting the pores and ensure permanent water shut-off treatment. To eliminate the danger of premature plug formation, stimulus-responsive materials were investigated. Considering that fractures are extremely hard-to-access places, the designed material should respond to a remotely applied stimulus, in order to achieve better control over plug formation.

The developed material consists of vinyl-functional polydimethylsiloxane (PDMS) microparticles and microcapsules with an encapsulated PDMS cross-linker. Due to reactions between the released cross-linker and vinyl groups on the PDMS microparticles’ surface, a covalently bonded elastomer plug is formed. The size of both components is adjusted to allow for creating the plug without affecting the pores. Control over cross-linking is achieved through an encapsulation process. Microcapsules prepared via a phase separation method are impermeable at 50°C, thereby eliminating premature plug formation. It is shown that after heating microcapsules to 120°C, the cross-linker is released from a poly(methyl methacrylate) (PMMA) shell. Moreover, gamma irradiation of the microcapsules decreases the Tg of the polymeric shell, changing the permeability of the microcapsules. Due to the irradiation process, microcapsules become permeable at lower temperatures, and a remotely applied activation has been achieved. Applying the alternating magnetic field (AMF) was another activation method investigated as part of this research. Magnetic nanoparticles, which generate heat on exposure to the AMF, were encapsulated successfully within the polymeric shell, and as a result, heating microcapsules when they are subjected to the AMF is possible. As an alternative to remote activation methods, solvent-flushing was examined, allowing for an investigation into the plug being cross-linked under high-pressure. Compressed material created a uniform, void-less structure capable of withstanding harsh conditions in reservoirs.
Renewability and emergy footprint at different spatial scales for innovative food systems in Europe

Food production is increasingly being challenged by limited resources of energy and land as well as by growing demand for food. In a future with less availability of fossil fuels, land area will become very important for capturing the flow-limited renewable resources. Energy assessment has been applied to calculate scale dependent indicators, which account for the land area needed, if agricultural systems were to be supported solely on renewable sources. These indicators are designated emergy footprints (EmFs) and expand the concept of support area defined previously in emergy accounting. The EmF (in ha) is calculated based on renewable empower densities which convert resource use into area equivalents able to capture renewable flows. The spatial division between on-site, local and non-local land areas applied in this study, identifies where the support area is located in order to apply a site-specific renewable empower density. A new indicator applying the EmF is the emergy overshoot factor, which estimates the ratio between EmF and the geographical system boundary (in ha). We apply this approach on three innovative food supply systems in Europe located at farms characterised by combining high diversity, reduced use of resources, nutrient cycling and local sales. The question is whether this type of food system may be considered sustainable from a resource use point of view measured as resource use efficiency by means of unit emergy value (UEV), renewability (R_{on-site} and R_{global}), direct and indirect occupation of land on different spatial scales (EmF and Emergy overshoot factor) and productivity per ha of the directly observed areas and the EmF area, respectively. Labour inputs constituted between 13 and 80 % of the total emergy flow. The proportion of resource use from renewable sources was between 31 and 60% when excluding the inputs of direct labour. The food system with the lowest UEV, excluding direct labour, had the highest emergy overshoot factor, which even exceeded the global average of seven. However, this system had the highest productivity. The system with the highest UEV, excluding direct labour, had the lowest overshoot factor. In conclusion, each food system strategy has its pros and cons and it depends on the priorities, which is judged the most sustainable from an emergy point of view. © 2015 Elsevier Ltd. All rights reserved.

Economic analysis, allied to process systems engineering tools, can provide useful insights about process techno-economic feasibility. More interestingly, rather than being used to evaluate specific process conditions, this techno-economic analysis can be turned upside down to achieve target values for the main process metrics, providing feedback to the research and development team and setting goals for experimental efforts. The present study proposes a methodology for performing such a "retro" techno-economic analysis. It consists of choosing the most important variables of the process and finding their threshold values and the correlation between them. To demonstrate the capabilities of the methodology, the production of succinic acid from sucrose was assessed. Through the use of this methodology, an infeasible region was identified and threshold values for the process variables were obtained. Although applied to a biochemical process, the methodology is general and can be applicable to all types of chemical processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidade Federal de Sao Carlos, Universidade Estadual de Maringá, Universidade Federal do Rio de Janeiro
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Rhamnogalacturonan I modifying enzymes: an update

Rhamnogalacturonan I (RGI) modifying enzymes catalyse the degradation of the RGI backbone and encompass enzymes specific for either the α1,2-bond linking galacturonic acid to rhamnose or the α1,4-bond linking rhamnose to galacturonic acid in the RGI backbone. The first microbial enzyme found to be able to catalyse the degradation of the RGI backbone, an endo-hydrolase (EC 3.2.1.171) derived from Aspergillus aculeatus, was discovered 25 years ago. Today the group of RGI modifying enzymes encompasses endo- and exo-hydrolases as well as lyases. The RGI hydrolases, EC 3.2.1.171–EC 3.2.1.174, have been described to be produced by Aspergillus spp. and Bacillus subtilis and are categorized
in glycosyl hydrolase families 28 and 105. The RGI lyases, EC 4.2.2.23–EC 4.2.2.24, have been isolated from different fungi and bacterial species and are categorized in polysaccharide lyase families 4 and 11. This review brings together the available knowledge of the RGI modifying enzymes and provides a detailed overview of biocatalytic reaction characteristics, classification, structure-function traits, and analyses the protein properties of these enzymes by multiple sequence alignments in neighbour-joining phylogenetic trees. Some recently detected unique structural features and dependence of calcium for activity of some of these enzymes (notably the lyases) are discussed and newly published results regarding improvement of their thermostability by protein engineering are highlighted. Knowledge of these enzymes is important for understanding microbial plant cell wall degradation and for advancing enzymatic processing and biorefining of pectinaceous plant biomass.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Silva, I. R. (Intern), Jers, C. (Intern), Meyer, A. S. (Intern), Mikkelsen, J. D. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.67 SJR 1.065 SNIP 1.269
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.069 SNIP 1.07 CiteScore 3.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.994 SNIP 1.248 CiteScore 2.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.819 SNIP 0.988 CiteScore 2.5
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.788 SNIP 0.836 CiteScore 2.12
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.934 SNIP 0.952 CiteScore 2.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.89 SNIP 1.023
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.028 SNIP 1.401
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.936 SNIP 1.098
Scopus rating (2007): SJR 1.381 SNIP 1.325
Scopus rating (2006): SJR 0.752 SNIP 0.898
Scopus rating (2005): SJR 0.685 SNIP 1.097
Scopus rating (2004): SJR 0.72 SNIP 1.043
Rheology of Supramolecular Polymers

Supramolecular polymers are a broad class of materials that include all polymers capable of associating via secondary interactions. These materials represent an emerging class of systems with superior versatility compared to classical polymers with applications in food stuff, coatings, cost efficient processes or biomedical areas. Design and development of supramolecular polymers using ionic, hydrogen bonding or transition metal complexes with tailored properties requires deep understanding of dynamics both in linear and non-linear deformations. While linear rheology is important to understand the dynamics under equilibrium conditions, extensional rheology is relevant during the processing or in the usage of polymers utilizing supramolecular associations for example, acrylic based pressure sensitive adhesives are subjected to extensional deformations during the peeling where strain hardening is often desirable. Such data is also needed to develop sophisticated multiscale models that can later be used for predicting the flow behavior and molecular dynamics of supramolecular networks. This thesis focuses on the experimental rheological study of two class of supramolecular polymers namely: (a) hydrogen bonding polymers, and (b) ionic bonding polymers (hereafter termed as ionomers). We study linear and non-linear rheology for a model system of entangled pure poly(n-butyl acrylate), PnBA, homopolymer and four poly(acrylic acid), PnBA-PAA, copolymers with varying AA side groups synthesized via hydrolysis of pure PnBA homopolymer. Second, we investigate the linear viscoelastic response of unentangled 2-ureido-4[1H]-pyrimidones (UPy) based supramolecular networks. Third, we investigate the rheological response of ionomers synthesized via condensation of sulfonated phthalates with poly(tetramethylene glycol)PTMO, both in non-linear shear and extensional flows. Finally, we study brittle fracture of the above ionomers in extensional flow.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Shabbir, A. (Intern), Hassager, O. (Intern), Skov, A. L. (Intern)
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Safeprops: A Software for Fast and Reliable Estimation of Safety and Environmental Properties for Organic Compounds
We present a new software tool called SAFEPROPS which is able to estimate major safety-related and environmental properties for organic compounds. SAFEPROPS provides accurate, reliable and fast predictions using the Marrero-Gani group contribution (MG-GC) method. It is implemented using Python as the main programming language, while the necessary parameters together with their correlation matrix are obtained from a SQLite database which has been populated using off-line parameter and error estimation routines (Eq. 3-6).

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Scale-up of industrial biodiesel production to 40 m³ using a liquid lipase formulation

In this work, we demonstrate the scale-up from an 80 L fed-batch scale to 40 m³ along with the design of a 4 m³ continuous process for enzymatic biodiesel production catalysed by NS-40116 (a liquid formulation of a modified Thermomyces lanuginosus lipase). Based on the analysis of actual pilot plant data for the transesterification of used cooking oil and brown grease, we propose a method applying first order integral analysis to fed-batch data based on either the bound glycerol or free fatty acid content in the oil. This method greatly simplifies the modelling process and gives an indication of the effect of mixing at the various scales (80L to 40m³) along with the prediction of the residence time needed to reach a desired conversion in a CSTR.

Suitable process metrics reflecting commercial performance such as the reaction time, enzyme efficiency and reactor productivity were evaluated for both the fed-batch and CSTR cases. Given similar operating conditions, the CSTR operation on average, has a reaction time which is 1.3 times greater than the fed-batch operation.

We also showed how the process metrics can be used to quickly estimate the selling price of the enzyme. Assuming a biodiesel selling price of 0.6 USD/kg and a one-time use of the enzyme (0.1% (w/w oil) enzyme dosage); the enzyme can then be sold for 30 USD/kg which ensures that that the enzyme cost is not more than 5% of the biodiesel revenue. This article is protected by copyright. All rights reserved
The objective of this paper is to systematically investigate the influences of different preparation methods on the properties of NiFe$_2$O$_4$ nanoparticles as oxygen carrier in chemical looping hydrogen production (CLH). The solid state (SS), coprecipitation (CP), hydrothermal (HT), and sol-gel (SG) methods were used to prepare NiFe$_2$O$_4$ oxygen carriers. Samples were characterized by X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Brunauer-Emmett-Teller (BET) surface area measurement, as well as Barrett-Joyner-Halenda (BJH) porosity test. The performance of the prepared materials was first evaluated in a TGA reactor through a CO reduction and subsequent steam oxidation process. Then a complete redox process was conducted in a fixed-bed reactor, where the NiFe$_2$O$_4$ oxygen carrier was first reduced by simulated biomass pyrolysis gas (24% H$_2$ + 24% CO + 12% CO$_2$ + N$_2$ balance), then reacted with steam to produce H$_2$, and finally fully oxidized by air. The NiFe$_2$O$_4$ oxygen carrier prepared by the sol gel method showed the best capacity for hydrogen production and the highest recovery degree of lattice oxygen, in agreement with the characterization results. Furthermore, compared to individual nickel ferrite particles, the mixture of NiFe$_2$O$_4$ and SiO$_2$ presented remarkably higher stability during 20 cycles in the fixed-bed reactor. The structural and morphological stability of samples after reactions was also examined by XRD, XPS, and SEM analyses.
Selective distribution of enzymes in a microfluidic reactor

Off stoichiometric thiol-ene mixtures are well suited for preparation of microfluidic devices with highly functional surfaces. Here a two stage process employing first thiol-ene chemistry (TEC) to prepare two opposite parts of a microfluidic system with a 30x30 mm reactor and subsequently a thiol-epoxy bonding was used to prepare a fully sealed microfluidic system. The reactor was surface functionalized in-situ with allyl glycidyl ether in different patterns (half-reactor, full-reactor, checkerboard structures) on the surface to provide a controlled distribution of epoxides. The method additionally enables the selective immobilization on either top-side or bottom-side or both sides of the reactor. Thereafter horseradish peroxidase was immobilized on the surface and activity tests illustrated how this distribution of the enzyme on the surface could be used to optimize the activity of the enzyme. The results were corroborated by CFD simulations.

Self-Healing, High-Permittivity Silicone Dielectric Elastomer

Currently used dielectric elastomers do not have the ability to self-heal after detrimental events such as tearing or electrical breakdown, which are critical issues in relation to product reliability and lifetime. In this paper, we present a self-healing dielectric elastomer that additionally possesses high dielectric permittivity and consists of an interpenetrating polymer network of silicone elastomer and ionic silicone species that are cross-linked through proton exchange between amines and acids. The ionically cross-linked silicone provides self-healing properties after electrical breakdown or cuts made directly to the material due to the reassembly of the ionic bonds that are broken during damage. The dielectric elastomers presented in this paper pave the way to increased lifetimes and the ability of dielectric elastomers to survive millions of cycles in high-voltage conditions.
Self-restoring polymer brushes under tribological stress and the biomedical applications

For biological and mechanical systems involving moving parts, surface slipperiness is often a critical attribute for their optimal functions. Surface grafting with hydrophilic polymers is a powerful means to render materials slippery in aqueous environment. In "inverted grafting-to approach", the hydrophilic polymer chains of amphiphilic diblock copolymers dispersed within a poly(dimethylsiloxane) (PDMS) network are selectively segregated upon exposure to aqueous solution. This allows formation of extremely stable brush-like polymer layers. Tribological application of inverted grafting-to approach was successfully demonstrated with PDMS-block-poly(acrylic acid) (PDMS-b-PAA) dispersed within thin PDMS films on PDMS blocks by showing friction coefficients (µ) of ca 10⁻² to 10⁻³, depending on the load, pH and buffer salinity in the absence of other external re-supply of PAA chains. Further manipulations of the thin PDMS film incorporating PDMS-b-PAA to optimize the tribological properties are presented. Lastly, first trials to employ PAA-grafted PDMS surface to generate in-vitro mucosae model are also presented and discussed.

General information
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Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Technical University of Denmark
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Pages: 1971-1976
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Main Research Area: Technical/natural sciences

Shear and Extensional Rheology of Polystyrene Melts and Solutions with the Same Number of Entanglements

We investigate the nonlinear shear and uniaxial extensional rheology of entangled polystyrene (PS) melts and solutions having the same number Z of entanglements, hence identical linear viscoelasticity. While experiments in extensional flows confirm that PS melts and solutions with the same Z behave differently, respective transient and steady data in simple shear over the largest possible range of rheometric shear rates (corresponding to Rouse-Weissenberg numbers from 0.01 to 40) demonstrate that melts and solutions exhibit identical behavior. Whereas the differences between melts and solutions in elongational flows are due to alignment induced friction reduction (more effective in melts than in solutions), in shear flows they disappear since the rotational component reduces monomeric alignment substantially. Recent molecular dynamics simulations of entangled polymers show that rotation induces molecular tumbling at high shear rates, and here a tube-based model involving tumbling effects is proposed in order to describe the response in shear. The main outcome is that tumbling can explain transient stress undershoot (following the overshoot) at high shear rates. Hence, the combination of tumbling in shear and friction reduction in extension successfully describes the whole range of experimental data and provides the basic ingredient for the development of molecular constitutive equations.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, University of Crete, University of Naples Federico II
Silicone elastomers with aromatic voltage stabilizers

A method to synthesise a polydimethylsiloxane-polyphenylmethylsiloxane (PDMS-PPMS) copolymer with electron-trapping effects has been developed utilising a quick hydrosilylation reaction at ambient temperature and crosslinking via hydrosilylation by a vinyl-functional crosslinker. The electrical breakdown strength, the storage modulus and the loss modulus of the elastomer were investigated, as well as the excitation energy from the collision between electron carriers and benzene rings in PDMS-PPMS copolymer was measured by UV-vis spectroscopy. The developed elastomers were inherently soft with enhanced electrical breakdown strength due to delocalized pi-electrons of aromatic rings attached to the silicone backbone. The dielectric relative permittivity of PDMS-PPMS copolymers remained between 2 to 3 with low conductivity and low dielectric loss as well as high storage moduli with low viscous loss, thereby maintaining the electro-mechanical integrity of the elastomer.

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: A Razak, A. H. (Intern), Skov, A. L. (Intern)
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Silicone elastomers with aromatic voltage stabilizers

Electrical breakdown causes short-circuiting of dielectric elastomers (DEs) resulting in irreversible destruction of the DE. The electrical field at which the un-actuated elastomer breaks down is known as the electrical breakdown strength. Numerous studies have been performed in order to obtain elastomers with high relative permittivity and low Young's modulus in order to increase the actuation performance at a given voltage, but the optimised elastomers often possess relatively low electrical breakdown strength. On the other hand, increasing the electrical breakdown strength of DEs allows for larger actuation due to the possibility of utilizing larger electrical fields.1,2 Many studies on electrical breakdown of pre-stretched DEs have been conducted, however less efforts have been focused on improving the electrical breakdown strength such as by blending in additives or by polymer structure modifications. In order to increase the electrical breakdown strength of polymers for e.g. the cable industry, additives like aromatic voltage stabilizers are used. Earlier works on using voltage stabilizers in polymers have mainly focused on polyethylene with the purpose of reducing power loss for high voltage insulation cables.3–5 As an alternative to utilise additives as voltage stabilizers, grafting aromatic compounds to silicone backbones may overcome the common problem of insolubility of the aromatic voltage stabilizer in the silicone elastomers due to phase separation. Preventing phase separation during preparation and during operation is a key requirement for long life-times of DEs.5

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Silicone elastomers with aromatic voltage stabilizers

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Authors: A Razak, A. H. (Intern), Skov, A. L. (Intern)
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Main Research Area: Technical/natural sciences
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Silicone elastomers with superior softness and dielectric properties

Dielectric elastomers (DEs) change their shape and size under a high voltage or reversibly generate a high voltage when deformed. The obstacle of high driving voltages, however, limits the commercial viability of the technology at present. Driving voltage can be lowered by decreasing the Young's modulus and increasing the dielectric permittivity of silicone elastomers. One such prominent method of modifying the properties is by adding suitable additives. [1] The major drawbacks for adding solid fillers are agglomeration and increasing stiffness which is often accompanied by the decrease of electrical breakdown and achievable strain.[2] In this work, three liquid additives - inert silicone oil, chloropropyl-functional silicone oil, and synthesized chloropropyl-functional copolymer - were blended into commercial silicone elastomers, and their properties were investigated. The functional groups were determined by NMR and morphology structures were investigated by optical microscopy. The resulting elastomers were evaluated with respect to their dielectric permittivity, tear and tensile strengths, as well as electrical breakdown. The breakdown strength increased at low amounts of additives whereas it decreased at larger amounts. The elastomers became increasingly soft with increasing addition of soft filler. Both inert and chloropropyl-functional silicone oils enhanced the molecular motions of the network substructures via dynamic dilution effects but the viscous losses also increased with increasing amount of silicone oils. Cross-linkable chloropropyl-functional copolymer offered a high level of mechanical integrity of the blended elastomers thus consequent low viscous losses. The dielectric permittivity of chloropropyl-functional blended elastomers increased greatly compared to the pristine commercial elastomer, while the dielectric losses remained at a low level. The increase in dielectric permittivity stemmed from the high dipole moment of the chloride groups. Furthermore, the alkyl chloride units yielded a larger free volume resulted in a less dense material with a lower Young's modulus.[3]

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Silicone elastomers with superior softness and dielectric properties

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General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Yu, L. (Intern), Madsen, F. B. (Intern), Zakaria, S. B. (Intern), Skov, A. L. (Intern)
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Main Research Area: Technical/natural sciences
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Silicone-modified graphene oxide fillers via the Piers-Rubinsztajn reaction

While graphene or graphene oxide can make significantimprovements in the properties of a wide variety of polymericmaterials, their incorporation can be challenged bycompatibility with the polymeric matrix. The modification of graphene oxide with silicones or silanes using the Piers-Rubinsztajn reaction improves dispersibility in nonpolar materials, including organic solvents and silicone pre-elastomers. A high loading (up to 10 wt %) of modified graphene oxide insilicone elastomers could be achieved, which resulted inenhanced mechanical performance and reduced gas permeability.

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
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Silicone rubbers for dielectric elastomers with improved dielectric and mechanical properties as a result of substituting silica with titanium dioxide

One prominent method of modifying the properties of dielectric elastomers (DEs) is by adding suitable metal oxide fillers. However, almost all commercially available silicone elastomers are already heavily filled with silica to reinforce the otherwise rather weak silicone network and the resulting metal oxide filled elastomer may contain too much filler. We therefore explore the replacement of silica with titanium dioxide to ensure a relatively low concentration of filler. Liquid silicone rubber (LSR) has relatively low viscosity, which is favorable for loading inorganic fillers. In the present study, four commercial LSRs with varying loadings of silica and one benchmark room-temperature vulcanizable rubber (RTV) were investigated. The resulting elastomers were evaluated with respect to their dielectric permittivity, tear and tensile strengths, electrical breakdown, thermal stability and dynamic viscosity. Filled silicone elastomers with high loadings of nano-sized titanium dioxide (TiO2) particles were also studied. The best overall performing formulation had 35 wt.% TiO2 nanoparticles in the POWERSIL® XLR LSR, where the excellent ensemble of relative dielectric permittivity of 4.9 at 0.1 Hz, breakdown strength of 160 V μm⁻¹, tear strength of 5.3 MPa, elongation at break of 190%, a Young’s modulus of 0.85 MPa and a 10% strain response (simple tension) in a 50 V μm⁻¹ electric field was obtained.

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Bibliographical note
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Simulation and multivariable optimization of post-combustion capture using piperazine

Piperazine presents a great potential to develop an energy efficient solvent based CO₂ post-combustion capture process. Recently 8 molal piperazine (PZ) has shown promising results, however it faces operational challenges due to limited solid solubility. The operating range can be extended by decreasing the concentration of PZ and/or increasing the lean loading. However, optimal process conditions must be determined accounting for heating and cooling demands plus solvent re-circulation. In this paper, we identify and generalize trends of performance for a broad range of operating conditions: 1.8-9 m PZ/kg water (molal) and 0.2-0.6 lean loading for absorption and desorption in both, open and closed-loop simulation. We pinpoint scenarios where intercooling significantly improves the performance of the post-combustion process. The energy penalty is minimized as part of the closed-loop multivariable optimization. The results are created in Aspen Plus using the hybrid CAPCO2 rate-based user model. This model includes precipitation when estimating the heat and mass transfer rates. The results show how the capture process needs to be operated up to 14% above the minimum achievable heat duty, to avoid clogging from solid formation. 5 m PZ is the most promising trade-off between energy efficiency and solid-free operation with a specific reboiler duty of 3.22 GJ/t CO₂ at 0.34 lean loading. The performance of the process can be further improved by assuming a minimum temperature of 30 °C which gives an optimal specific reboiler duty of 3.09 GJ/t CO₂ (8 m PZ, 0.334 lean loading) for conditions without advanced heat integration.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.499 SNIP 2.633 CiteScore 6.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Solubility Measurements and Modeling of Zinc, Lead and Iron Sulfides at High Temperatures and High Pressures

Solubility measurements of sulfides in aqueous solutions are necessary to understand the behaviour of these scaling minerals in geothermal and oil reservoirs. The low solubility levels of Zinc Sulfide (ZnS), Lead Sulfide (PbS) and Iron Sulfide (FeS) make the solubility measurements a challenging task. Consequently existing data are rare and scattered. The aim of this work is to develop a reliable experimental procedure and to measure solubility of sulfides at high temperature and pressures. Additionally the experimental data are used for estimation of the solid-liquid equilibrium using the Extended UNIQUAC model.

The experimental determination of the solubility of ZnS, PbS and FeS is carried out at temperatures up to 200°C and pressures up to 60 bars. The minerals in their pure form are added to ultra-pure water previously degassed with nitrogen. The aqueous solution is prepared in a reduced oxygen atmosphere to avoid the risk of oxidation of sulfide minerals. The solution is kept in an equilibrium cell at constant temperature and pressure with continuous stirring. The concentration of Zn$^{2+}$, Pb$^{2+}$, Fe$^{2+}$ and S$^{2-}$ are measured using Inductively Coupled Plasma Optical Emission spectrometry (ICP-OES) as analytical technique.

The solid-liquid equilibria is calculated using the Extended UNIQUAC model. The Extended UNIQUAC model is a local composition model and features several advantages compared to other models when describing the behaviour of aqueous electrolytes systems and it was presented by Thomsen and Rasmussen in 1999. The model accounts for the dependency of the solubility on pressure and temperature. The pressure parameters were proposed by Villafáñila et al. (2005; 2006) on their study on sulfate scaling minerals. The parameter estimation of the model is carried out based on the experimental data produced in our laboratory. The results show that the Extended UNIQUAC model can correlate the solubility data for sulfides within experimental accuracy.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Solubility Modeling of the Binary Systems Fe(NO$_3$)$_3$–H$_2$O, Co(NO$_3$)$_2$–H$_2$O and the Ternary System Fe(NO$_3$)$_3$–Co(NO$_3$)$_2$–H$_2$O with the Extended Universal Quasichemical (UNIQUAC) Model

Solubility modeling in the binary system Fe(NO$_3$)$_3$–H$_2$O, Co(NO$_3$)$_2$–H$_2$O and the ternary system Fe(NO$_3$)$_3$–Co(NO$_3$)$_2$–H$_2$O is presented. The extended UNIQUAC model was applied to the thermodynamic assessment of the investigated systems. The model parameters obtained were regressed simultaneously using the available databank but with more experimental points, recently published in the open literature. A revision of previously published parameters for the cobalt ion and new parameters for the iron(III) nitrate system are presented. Based on this set of parameters, the equilibrium constants of hydrates are determined. The model represents the experimental data with good accuracy from the freezing point region to the boiling points of the solutions.
Solvent selection methodology for pharmaceutical processes: Solvent swap

A method for the selection of appropriate solvents for the solvent swap task in pharmaceutical processes has been developed. This solvent swap method is based on the solvent selection method of Gani et al. (2006) and considers additional selection criteria such as boiling point difference, volatility difference, VLE phase diagram analysis, and azeotropic information that are particularly important for the solvent swap task. The method employs a solvent-swap database together with calculation tools for properties–functions of solvents. The database contains solvents that are commonly used in pharmaceutical processes as well as new solvent swap alternatives. The method takes into account process considerations such as batch distillation and crystallization to achieve the swap task. Rigorous model based simulations of the swap operation are performed to evaluate and compare the performance of the selected solvents. A guide and a software tool that allow the fast and reliable identification of the swap solvent have been developed. The main features and the applicability of the method are highlighted through several practical examples.
Sources and propagation of uncertainty in N2O model predictions

General information
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Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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Sourcing and bioprocessing of brown seaweed for maximizing glucose release
The research undertaken for this PhD thesis has been part of a larger research program “The MacroAlgaeBiorefinery – sustainable production of third generation (3G) bioenergy carriers and high value aquatic fish feed from macroalgae (MAB3)”. The research has been based on the overall hypothesis that brown seaweeds represent a huge unexploited bioresource of the sea which can be upgraded to energy carriers via degradation to fermentable sugars. The research in the PhD thesis has aimed at optimizing pretreatment and enzymatic saccharification of Saccharina latissima and Laminaria digitata to release maximum levels of glucose. The first requirement was to develop a robust methodology, including acid hydrolysis and analytical composition analysis, to quantitatively estimate the carbohydrate composition of the brown seaweeds. The monosaccharide composition of four different samples of brown seaweeds Laminaria digitata and Saccharina latissima were compared by different high performance anion exchange chromatography (HPAEC) methods after 3 different acid hydrolysis treatments or a cellulase treatment. HPAEC analysis with pulsed amperometric detection (PAD) preceded 2-step pretreatment with 72 % sulfuric acid (H2SO4) for 1 h at 30 °C and followed by 4 % H2SO4 at 120 °C for 40 min allowed quantitative determination of the carbohydrate composition of brown seaweed. The chemical composition of brown seaweed varied mainly in regard to the season but differed also with respect to species, location, between the years and even within the population. Concentrations of ash and protein levels varied inversely to the carbohydrate levels, and total carbohydrate concentration varied seasonally,
in particular through the storage of carbohydrates glucose and mannitol. Generally, alginate was the most abundant carbohydrate at all sites from December to summer with up to 36 % w/wDM by weight before glucose levels were at least at the same magnitude. Total alginate concentration was relatively independent of seasonal changes but mannuronic (M) and guluronic acid (G) differed strongly throughout the year. M/G ratios varied regarding season, species or location from 1.3 to 3.6 but without a general pattern. The highest concentrations of glucan were found in August for wild growing L. digitata from the North Sea, with the glucose potential lying >50 % w/wDM for three sequential years (2012-2014) accompanied by mannitol levels of about 10 % w/wDM and low ash levels of 10-11 % w/wDM. Generally spoken, glucose levels of L. digitata appeared to be superior to those of S. latissima. Cultivation of S. latissima in the Limfjorden, Denmark to obtain high glucan levels was not possible due to the incidence of biofouling in the summer. The average N-to-protein conversion factor was 3.7 but ranged from 2.1 to 5.9. Hence, application of a common factor cannot be recommended since total nitrogen content was more variable than the protein content. Post washing L. digitata harvested from the Danish North Sea in August 2012 had a total organic matter of 84 % mostly accounted for glucose (51 % w/wDM), including a smaller contribution of mannitol (8 % w/wDM), making this material an ideal feedstock for biocatalytical processing to achieve maximum glucose release. The influence of milling as pretreatment to enhance enzymatic degradation was studied on the glucan rich L. digitata (North Sea, August 2012). Wet refiner milling, using rotating disc distances of 0.1-2 mm, generated differently sized particle populations with particles having decreasing average surface area (100-0.1 mm2) with increased milling severity. Milling with disc distances below the thickness of the algae (≤1 mm) increased the particle volume of the milled seaweed slurries and higher milling severity (lower rotating disc distance) also induced higher carbohydrate solubilization from the material, particularly for glucan and mannitol. However, particle size diminution did not improve the enzymatic glucose release. Milling was thus not required for enzymatic saccharification because all available glucose was released even from unmilled material during the combined treatment of alginate lyase and the cellulase preparation Cellic®CTec2. Apparently, the alginate lyase (Sigma Aldrich) activity catalyzed the cleavage of alginate on the substrate, which both decreases the viscosity of the substrate alginate and catalytically solubilizes the alginate to provide access to the glucan in the brown seaweed cell wall matrix. The impact of alginate lyase in addition to cellulase on the brown seaweed degradation was studied further for L. digitata degradation. Therefore, two bacterial alginate endo-lyases (EC 4.2.2.-) from Sphingomonas sp. (SALy) and Flavobacterium sp. (FALy) were selected for heterologous, monocomponent expression in Escherichia coli. The optimal pH range for SALy was pH 5.5-7.0 with optimum at pH 6. The optimum for FALy and the commercially available alginate lyase from Sigma Aldrich (SigmALy) was pH 7.5. The investigated reaction temperatures of 30-50 °C had no influence on the activity. The thermal stability was reduced above 50 °C, for SigmALy above 40 °C. The FALy preferred poly-mannuronic acid as substrate, but also exhibited activity on poly-guluronic acid, whereas SALy had higher activity on poly-guluronic acid and SigmALy was only active on poly-guluronic acid. Subsequently, the alginate lyases were applied together with the commercial, fungiely derived cellulase preparation Cellic®CTec2 at pH 6 and 40 °C on the glucan rich L. digitata. A decrease in viscosity decrease ensued in the initial minutes while alginate degradation occurred primarily within the first 1-2 hours of reaction. The level of released mannuronic acid blocks was inversely proportional to the glucose release indicating that the degradation of mannuronic acid blocks inhibited the cellulase catalyzed glucose release from L. digitata. Only the selective activity of SigmALy on guluronic acid enabled a 90 % glucose release within 8 hours by the cellulase preparation Cellic®CTec2. Nevertheless, combined alginate lyase and cellulase treatment for 24 hours released all potential glucose regardless of the applied lyase. Treatment with a mixture of 1 % w/wDM SigmALy and 10 % v/wDM Cellic®CTec2 at pH 5 and 40 °C released the available glucose during 8 hours. Two-thirds of the glucose was released with lower enzyme loading. Simple application of only the cellulase preparation enabled the release of only half of the present glucose after 8 h. Analysis after the enzymatic treatment indicated a potential extraction of proteins from the solid residue and the sulfated polysaccharide fucoidan solubilized in the saccharified liquid. The results of this PhD study demonstrated that brown seaweed can be completely degraded enzymatically by combined cellulase and alginate lyase treatment after milling. The work also showed, that bio-refining of brown seaweed with current state of art technology is highly dependent on the cultivation, in particular growth site and season, of a suitable feedstock for achieving maximal glucan content and in turn allowing maximum glucose release.
Sourcing and bioprocessing of brown seaweed for maximizing glucose release
Source: PublicationPreSubmission
Source-ID: 127442032
Publication: Research › Ph.D. thesis – Annual report year: 2016

Statistical model semiquantitatively approximates arabinoxyloligosaccharides' structural diversity
A statistical model describing the random distribution of substituted xylopyranosyl residues in arabinoxyloligosaccharides is suggested and compared with existing experimental data. Structural diversity of arabinoxyloligosaccharides of various length, originating from different arabinoxylans (wheat flour arabinoxylan (arabinose/xylose, A/X = 0.47); grass arabinoxylan (A/X = 0.24); wheat straw arabinoxylan (A/X = 0.15); and hydrothermally pretreated wheat straw arabinoxylan (A/X = 0.05)), is semiquantitatively approximated using the proposed model. The suggested approach can be applied not only for prediction and quantification of arabinoxyloligosaccharides' structural diversity, but also for estimate of yield and selection of the optimal source of arabinoxylan for production of arabinoxyloligosaccharides with desired structural features.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Dotsenko, G. (Intern), Nielsen, M. K. (Intern), Lange, L. (Intern)
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Scopus rating (2014): SJR 0.638 SNIP 0.856 CiteScore 2.01
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.773 SNIP 1.017 CiteScore 2.2
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.76 SNIP 1.062 CiteScore 2.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.722 SNIP 0.868
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.883 SNIP 1.031
Web of Science (2009): Indexed yes
Statistical optimization of operating parameters for CSTR bioprocesses: the case study of glycerol conversion

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, PILOT PLANT
Authors: Varrone, C. (Intern), Skiadas, I. V. (Intern), Gavala, H. N. (Intern)
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Main Research Area: Technical/natural sciences
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Bibliographical note
Sustain Abstract R-6
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Stepwise extraction of Lepidium sativum seed gum: Physicochemical characterization and functional properties
Cress seed gum (CSG) was fractionated using stepwise extraction with water, yielding three fractions (F1, F2, F3) whose average molecular weights ranged from 863 to 1080 kDa. The chemical composition (monosaccharide, ash, moisture, CHN and uronic acid contents) and molecular weight of the fractions varied significantly. Generally, the major identical peaks of FT-IR spectra for three fractions and whole cress seed gum were similar. The results of DSC and TGA indicated that F3 had the highest thermal stability and considering the initial decomposition temperature, the decreasing order of thermal stability was F3 > F2 > F1. Cress seed gum and its fractions exhibited non-Newtonian shear thinning behavior which the Herschel-Bulkley model was successfully described the steady shear flow behavior of samples, and apparent viscosity followed the order of F3 > F2 > F1. F3 exhibited the best surface tension reducing ability compared to other fractions and CSG. All the samples had good emulsifying capability (>97%) and stability(>96%). The emulsion capacity increased slightly along the series of F1, F2 and F3, whereas, emulsion stability decreased along the same series. CSG and F3 showed the highest and the lowest foaming capacity and stability, respectively. © 2016 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Shahid Beheshti University of Medical Sciences, Ferdowsi University of Mashhad
Stress relaxation following uniaxial extension of polystyrene melt and oligomer dilutions

The filament stretching rheometer has been used to measure the stress relaxation following the startup of uniaxial extensional flow, on a narrow molar mass distribution (NMMD) polystyrene melt and styrene oligomer dilutions thereof. All samples used here were characterized in molecular weight, mechanical spectroscopy, and constant strain rate uniaxial extension in the work of Huang et al. [Macromolecules 46, 5026–5035 (2013); ACS Macro Lett. 2, 741–744 (2013)]. The stress relaxation following the steady extensional stress was measured on a 285 kg/mole NMMD polystyrene and two 1.92 kg/mole styrene oligomer dilutions thereof [PS-285k, PS-285k/2k-72, and PS-285k/2k-44 in the work of Huang et al. [Macromolecules 46, 5026–5035 (2013)]. The two dilutions contained 28 and 56 wt. % oligomer, respectively. Further, the stress relaxation on a 545 kg/mole NMMD polystyrene diluted with 48 wt. % 0.972 kg/mole styrene oligomer [PS-545k/1k-52 in the work of Huang et al. [ACS Macro Lett. 2, 741–744 (2013)] was measured as well. All the terminal relaxations could be predicted by a Doi and Edwards, e.g., pure configurational, type of model. At smaller time scales, agreement with a molecular stress function type of constitutive representation was observed for all measured relaxations. VC 2016 The Society of Rheology.
We present start-up of uniaxial extension followed by stress relaxation experiments of a bi-disperse 50\% by weight blend of 95k and 545k molecular weight polystyrene. We also show, for comparison, stress relaxation measurements of the polystyrene melts with molecular weight 95k and 545k, which are the components of the bi-disperse melt. The measurements show three separated relaxation regimes: a fast regime, a transition regime, and a slow regime. In the fast regime, the orientation of the long chains is frozen and the stress relaxation is due to stretch relaxation of the short chains primarily. Conversely in the slow regime, the long chains have retracted and undergo relaxation of orientation in fully relaxed short chains.
Structure, functionality and tuning up of laccases for lignocellulose and other industrial applications

Laccases (EC 1.10.3.2) are copper-containing oxidoreductases that have a relatively high redox potential which enables them to catalyze oxidation of phenolic compounds, including lignin-derived phenolics. The laccase-catalyzed oxidation of phenolics is accompanied by concomitant reduction of dioxygen to water via copper catalysis and involves a series of electron transfer reactions balanced by a stepwise re-oxidation of copper ions in the active site of the enzyme. The reaction details of the catalytic four-copper mechanism of laccase-mediated catalysis are carefully re-examined and clarified. The substrate range for laccase catalysis can be expanded by means of supplementary mediators that essentially function as vehicles for electron transfer. Comparisons of amino acid sequences and structural traits of selected laccases reveal conservation of the active site trinuclear center geometry but differences in loop conformations. We also evaluate the features and regions of laccases in relation to modification and evolution of laccases for various industrial applications including lignocellulosic biomass processing.
Surface characterization of activated chalcopyrite particles via the FLSmidth ROL process. Part 1: Electron microscope investigations

Because of its unique semiconductor properties, the world's most abundant copper mineral (chalcopyrite) is refractory with respect to atmospheric leaching using traditional ferric sulfate lixiviants. A novel approach to address this issue – conducted at FLSmidth – utilizes a mechanochemical Rapid Oxidative Leach (ROL) assisted by a Stirred Media Reactor (SMRt). Due to the elimination of much of the surface passivation problems associated with atmospheric leaching, this process is able to attain copper recoveries >97% in under 6 hours. An optional, rapid preconditioning step uses minute quantities of copper(II) to dope the semiconductor lattice and thereby "activate" the chalcopyrite, thereby reducing leach times below 2 hours (>98% recovery). Because the activation plays a major role in accelerating the leaching step, it is critical to understand the nature of this intermediate and its part in the ROL process. The current work presents results from electron microscope investigations of surface-activated particles.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), FLSmidth USA Inc.
Authors: Karcz, A. P. (Intern), Damø, A. J. (Intern), Illerup, J. B. (Intern), Rocks, S. (Ekstern), Dam-Johansen, K. (Intern), Chaiko, D. (Ekstern)
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Sustainable Chemical Process Development through an Integrated Framework
This paper describes the development and the application of a general integrated framework based on systematic model-based methods and computer-aided tools with the objective to achieve more sustainable process designs and to improve the process understanding. The developed framework can be applied to a wide range of problems, including the design of new processes as well as retrofit of existing batch-continuous production systems. The overview of the framework together with results from two case studies is presented to highlight the key aspects and the applicability of the framework. These case studies involve multiphase reaction systems for the synthesis of active pharmaceutical ingredients.

General information
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Authors: Papadakis, E. (Intern), Kumar Tula, A. (Intern), Anantpinijwatna, A. (Intern), Babi, D. K. (Intern), Gani, R. (Intern)
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Sustainable DME synthesis-design with CO2 utilization

Minimizing CO2 emission, while achieving economic feasibility in CO2 utilization for producing valuable chemicals is a challenging problem, as reported in recent studies. Due to its high Cetane number, clean-burning, and non-toxic, DME is a promising fuel alternative, and therefore, potentially valuable chemical that can be produced via thermochemical CO2 conversion reactions. The aim of this study is to identify the most promising processing route for sustainable production of DME in terms of CO2 emission, economic indicators and sustainable indicators. The three processing routes are generated: (A) dry reforming step, methanol synthesis step, and methanol dehydration step; (B) CO2 hydrogenation step followed by methanol dehydration step; and (C) dry reforming step followed by direct DME synthesis step. Starting with a base-case design, the process flow sheets for the three routes are studied in detail to identify the process bottlenecks or hot-spots. Alternatives addressing the hot-spots are generated to identify the processing route with the best potential. The results indicate that processing route-B gives the highest CO2 consumption; nevertheless, this route is not feasible in terms of economic factors due to the negative rate of return. The final selection, however, depends on a trade-off between CO2 consumption and economic sustainability indicators. In principle, for all three alternatives are more sustainable options.
Distillation is an energy intensive operation in chemical process industries. There are around 40,000 distillation columns in operation in the US, requiring approximately 40% of the total energy consumption in US chemical process industries. However, analysis of separations by distillation has shown that more than 50% of energy is spent in purifying the last 5-10% of the distillate product. Membrane modules on the other hand can achieve high purity separations at lower energy costs, but if the flux is high, it requires large membrane area. A hybrid scheme where distillation and membrane modules are combined such that each operates at its highest efficiency, has the potential for significant energy reduction without significant increase of capital costs. This paper presents a method for sustainable design of hybrid distillation-membrane schemes with guaranteed reduction of energy consumption together with two illustrative examples.
SYNERON – An Alternative Approach to the Production of Biofuels

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, PILOT PLANT
Authors: Asimakopoulos, K. (Intern), Grimalt Alemany, A. (Intern), Gavala, H. N. (Intern), Skiadas, I. V. (Intern)
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Synthesis and characterization of UV photocrosslinkable hydrogels with poly(N-vinyl-2-pyrrolidone): Determination of the network mesh size distribution

Hydrogels of poly(n-vinyl-2-pyrrolidone) were produced by UV irradiation of aqueous solutions of the polymer in presence of hydrogen peroxide, used as initiator. The mechanical and the nanostructural properties of the gels were characterized by a combination of experimental techniques including rheology, low field nuclear magnetic resonance spectroscopy (LF-NMR), and small angle X-ray scattering. Different irradiation doses as well as polymer and initiator concentrations were tested in the characterization. The study elucidates the relationship between different methods to estimate the mesh size of the gel polymeric network. Moreover, a novel correlation model was developed based on Chui and Scherer theories for the interpretation of LF-NMR dataset of polymer solutions and networks.

General information
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Organisations: Department of Micro- and Nanotechnology, Nanoprobes, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics, University of Trieste, National Research Council of Italy
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Web of Science (2017): Indexed Yes
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.423 SNIP 0.706 CiteScore 1.63
BFI (2014): BFI-level 1
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Scopus rating (2012): SJR 0.662 SNIP 1.022 CiteScore 1.62
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.374 SNIP 0.861 CiteScore 1.03
ISI indexed (2011): ISI indexed no
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Scopus rating (2010): SJR 0.261 SNIP 0.465
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.292 SNIP 0.424
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.218 SNIP 0.476
Scopus rating (2007): SJR 0.198 SNIP 0.406
Scopus rating (2006): SJR 0.214 SNIP 0.333
Synthesis of preliminary system designs for offshore oil and gas production

The present work deals with the design of oil and gas platforms, with a particular focus on the development of integrated and intensified petroleum processing plants. It builds on a superstructure based approach that includes all the process steps, transformations and interconnections of relevance, to generate and compare a large number of alternatives. The superstructure is formulated based on engineering knowledge and is coupled to process models developed in Aspen and Matlab, together with multi-objective optimisation routines and uncertainty assessments. It takes actual measurements from North Sea fields and three petroleum compositions as starting points. The significance of the uncertainties associated with the feed properties, and the capital costs, taxes and lifetime, is assessed. The results indicate that (i) the system performance strongly depends on the level of mass integration within the platform, (ii) the oil and gas recoveries are markedly impacted by the number of separation stages and heat exchangers, and (iii) disregarding the interactions between the several plant sections lead to sub-optimum solutions. The application of this framework proves to be useful for eliminating inadequate configurations and screening potentially novel solutions at early stage designs, with respect to technical, energetic and economic criteria.

General information

State: Published
Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Nguyen, T. (Intern), Sin, G. (Intern), Elmegaard, B. (Intern)
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Systematic design of an optimal control system for the SHARON-Anammox process

A systematic design of an optimal control structure for the SHARON-Anammox nitrogen removal process is studied. The methodology incorporates two novel features to assess the controllability of the design variables candidate for the
regulatory control layer: (i) H- control method, which formulates the control problem as a mathematical optimization problem, and (ii) close-loop disturbance gain (CLDG) plots. It is shown that the methodology is especially appropriate for bioreactors. The solution of the mixed sensitivity stacked H control problem ranked the combinations of controlled variables (CVs). The best candidates to CVs were paired with the manipulated variables using the relative gain array. The proposed control structure was further analyzed and verified for disturbance rejection using the CLDG plots. The optimal pairing of CVs with the actuators (kLa and acid/base addition) is found to be dissolved oxygen (DO) and pH in the SHARON reactor. Furthermore, to relate the controller actions to process operation objective, nitrogen removal efficiency, two cascade control systems are designed. The first cascade loop controls TNN/TAN ratio in the influent to the Anammox reactor by adjusting the set point for DO in the regulatory layer, while the second cascade loop controls the nitrogen removal efficiency (i.e. effluent TNN and TAN) by adjusting the TNN/TAN ratio at the effluent of the SHARON reactor. The control system is evaluated and benchmarked using a set of realistic dynamic scenario simulations, demonstrating that the different control strategies successfully maintain stable and high nitrogen removal efficiency. The nested cascade control structure shows the best performance, removing up to 95% of the influent ammonia. Both the control design methodology and the resulting optimal control structures are expected to contribute to stable operation and control of these emerging nitrogen removal technologies.

General information
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Authors: Valverde Perez, B. (Intern), Mauricio Iglesias, M. (Intern), Sin, G. (Intern)
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.521 SNIP 2.735 CiteScore 3.92
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.507 SNIP 2.607 CiteScore 3.47
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.563 SNIP 2.954 CiteScore 3.39
ISI indexed (2012): ISI indexed yes
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Scopus rating (2011): SJR 1.316 SNIP 2.59 CiteScore 2.9
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 1.305 SNIP 2.203
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Scopus rating (2009): SJR 1.282 SNIP 2.772
Systematic design of membership functions for fuzzy-logic control: A case study on one-stage partial nitritation/anammox treatment systems

A methodology is developed to systematically design the membership functions of fuzzy-logic controllers for multivariable systems. The methodology consists of a systematic derivation of the critical points of the membership functions as a function of predefined control objectives. Several constrained optimization problems corresponding to different qualitative operation states of the system are defined and solved to identify, in a consistent manner, the critical points of the membership functions for the input variables. The consistently identified critical points, together with the linguistic rules, determine the long term reachability of the control objectives by the fuzzy logic controller. The methodology is highlighted using a single-stage side-stream partial nitritation/Anammox reactor as a case study. As a result, a new fuzzy-logic controller for high and stable total nitrogen removal efficiency is designed. Rigorous simulations are carried out to evaluate and benchmark the performance of the controller. The results demonstrate that the novel control strategy is capable of rejecting the long-term influent disturbances, and can achieve a stable and high TN removal efficiency. Additionally, the controller was tested, and showed robustness, against measurement noise levels typical for wastewater sensors. A feedforward-feedback configuration using the present controller would give even better performance. In comparison, a previously developed fuzzy-logic controller using merely expert and intuitive knowledge performed worse. This proved the importance of using a systematic methodology for the derivation of the membership functions for multivariable systems. These results are promising for future applications of the controller in real full-scale plants. Furthermore, the methodology can be used as a tool to help systematically design fuzzy logic control applications for other biological processes.
Systematic design of optimal control systems for WWTPs: case study of the SHARON-Anammox process

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Systematic, efficient and consistent LCA calculations for chemical and biochemical processes
Life Cycle Assessment or LCA is a technique, which is applied for the study and evaluation of quantitative environmental impacts through the entire life cycle of products, processes or services in order to improve and/or evaluate the design of existing as well as new processes. The LCA factors can be used to identify and to improve the process environmental hotspots in order to make the process more sustainable. To complete the sustainable development of a process design, it is therefore necessary to consider both economic and environmental aspects. For this purpose, the LCSoft, a tool for systematic and consistent calculation of LCA factors has been developed (Supawanich et al., 2015). LCSoft integrates with other tools such as process simulation (PROII/ASPEN), ECON (economic analysis) and SustainPro (sustainability analysis) and provides for a specified boundary, all the established LCA factors. In this paper, new features that have widened the application range of LCSoft are presented together with evaluation of their performance. More specifically, this research focuses on improvements of the software performance in terms of extension of the LCI database and new calculation options that allow a wider coverage of chemical and biochemical processes. Improvements of LCIA calculations and eco-efficiency evaluation are introduced. Also, a new model for photochemical ozone formation has been developed and implemented. Performance of LCSoft in terms of accuracy and reliability is compared with another well-known LCA-software, SimaPro for a biochemical process – the production of bioethanol from cassava rhizome. The results show a very good match of new added impact categories. Also, the results from a new feature in LCSoft, which is eco-efficiency evaluation, are presented.

General information
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Systematic framework for carbon dioxide capture and utilization processes to reduce the global carbon dioxide emissions

In the year 2013, 9.5 billion metric tons of carbon dioxide gas was emitted into the air, and each year this amount is increasing [1]. Carbon dioxide emissions are of particular concern as they represent 80% of greenhouse gas emissions and therefore are a large contributor to global warming. Among the two approaches that are currently being investigated, carbon capture and storage (CCS) and carbon capture and utilization (CCU) [1] to address this issue, the later approach is more promising as it reuses captured carbon dioxide, as a fuel, reactant, solvent, and others, to produce valuable products. There is not only a need for technologies for capture and utilization, via conversion, but also there are numerous questions that need to be resolved. For example, which higher value chemicals can be produced, what are their current demands and costs of production, and how much of the captured carbon dioxide would be utilized? Also, how much carbon dioxide would be indirectly generated due to the capture and utilization efforts? Can the regulated carbon dioxide emission reduction targets be achieved only through the CCU and/or CCS efforts? Therefore, there is a need for a systematic computer-aided framework through which the issue of global carbon dioxide emissions can be investigated in terms of different available capture-utilization technologies, solution methods, and benefit scenarios, with the objective to determine more sustainable solutions within an appropriate application boundary. The framework would need to provide, amongst other options: useful data from in-house databases on carbon dioxide emission sources; mathematical models from a library of process-property models; numerical solvers from library of implemented solvers; and, work-flows and data-flows for different benefit scenarios to be investigated.

It is useful to start by developing a prototype framework and then augmenting its application range by increasing the contents of its databases, libraries and work-flows and data-flows. The objective is to present such a prototype framework with its implemented database containing collected information-data on various carbon dioxide emission sources and available capture-utilization technologies; the model and solution libraries [2]; and the generic 3-stage approach for determining more sustainable solutions [3] through superstructure (processing networks) based optimization – adopted for global carbon dioxide emission problems. More specifically, the prototype framework and the three-stage approach adopted for systematic and sustainable design of carbon capture and utilization processes incorporates (i) process synthesis stage, the determination of a processing path from a network of alternatives; (ii) process design, the design and analysis of a process or generated processing path in terms of process "hot-spots" or deficiencies to set design targets for improvement; and (iii) innovative and more sustainable design, determination of solutions matching the design targets. In this way, the starting point is an analysis of the current carbon dioxide emission status and the end point is an analysis of the more sustainable solutions in terms of one or more carbon dioxide benefit scenarios.

The developed framework contains a database constructed based on a developed knowledge representation structure, which has collected data on carbon dioxide emission sources, capture technologies, carbon dioxide-based reaction paths, and known utilization technologies leading to various products. The database currently has 5 carbon dioxide emission sources, 3 capture technologies, 10 conversion routes leading to 8 products, and over 50 reaction paths for many more products. The framework also integrates a software tool (the Super-O interface [2]) containing a library of process models and links to numerical solvers that enables the generation of processing networks (superstructure) and the determination of the optimal processing route. Finally, the framework has access to, a collection of tools for analysis, such as economic analysis, sustainability and life cycle assessment, and links to detailed process simulation (process simulators). Following the work-flow and data-flow implemented in the framework, data for the carbon capture and utilization alternatives are retrieved from the database and linked to form a network using the interface tool, Super-O. For each alternative, models for economic and environmental impacts are available; the promising utilization products considered are methanol, dimethyl carbonate, and succinic acid. The optimal utilization process (or processes) is determined via a superstructure-based method (using solvers in GAMS). Then, the carbon dioxide emission values for the utilization routes are compared with the current industrial production routes for the listed products in order to identify those that have zero or negative emission values (objective function). Subsequently, the identified utilization processes are designed rigorously and further improved with unique technology and integration options. Using this approach, the utilization processes for methanol, dimethyl carbonate and succinic acid give the following interesting result: by converting at least 70% (methanol), 40% (dimethyl carbonate) and 20% (succinic acid) of the current industrial processes to the corresponding utilization processes, the emissions from these processes can be neutralized, representing over 100 million metric tons of emissions that are neutralized. Note that the issue of product demand increase has not been considered. Also, on a global scale, this reduction of carbon dioxide emissions represents a very small but very valuable reduction. A more complete sustainability analysis is needed to enlarge the boundary of the analysis; for example, the boundary can change in terms of reduction of non-renewable resources and the use of renewable energy sources, as well as more efficient and sustainable designs of current production routes. While a combination of methods is needed to globally address carbon dioxide emissions and other aspects of sustainability, this systematic approach to designing carbon capture and utilization processes shows the capacity for such processes to reduce emissions and improve sustainability while producing valuable products. The current prototype framework with its implemented methods and tools is a small but important step.

Collaboration and integration of data, methods and tools is necessary to provide a more sustainable solution to the global carbon dioxide emission problem.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, Technical University of Denmark
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Systematic Integrated Process Design and Control of Binary Element Reactive Distillation Processes

In this work, integrated process design and control of reactive distillation processes is considered through a computer-aided framework. First, a set of simple design methods for reactive distillation column that are similar in concept to non-reactive distillation design methods are extended to design-control of reactive distillation columns. These methods are based on the element concept where the reacting system of compounds is represented as elements. When only two elements are needed to represent the reacting system of more than two compounds, a binary element system is identified. It is shown that the same design-control principles that apply to a non-reacting binary system of compounds are also valid for a reactive binary system of elements for distillation columns. Application of this framework shows that designing the reactive distillation process at the maximum driving force results in a feasible and reliable design of the process as well as the controller structure.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana
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Main Research Area: Technical/natural sciences

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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 1.004 SNIP 1.234 CiteScore 2.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
In this work, integrated process design and control of reactive distillation processes that involve multiple elements (more than two) is addressed through a computer-aided hierarchical decomposition-based framework. Multiple elements are encountered for reactive systems when four or more compounds (including inert compounds) are encountered. The reactive distillation design methods and tools which are similar in concept to design of binary non-reactive distillations and binary reactive distillations are used for design of multi-element reactive distillation processes, such as driving force approach. The methods that are used in this work are based on equivalent binary element concept. This concept provides the representation of a multi-element system in terms of two key elements, light key and heavy key elements. First, the reactive distillation column is designed using the equivalent binary element driving force approach. Next, through analytical, steady-state and closed-loop dynamic analysis it is verified that the control structure, disturbance rejection and energy requirement of the reactive distillation column is better than any other operation point that is not at the maximum driving force. Furthermore, it is shown that the design at the maximum driving force can be both controlled using simple controllers such as PI as well as advanced controllers such as MPC.

**Systematic Integrated Process Design and Control of Reactive Distillation Processes Involving Multi-elements**

In this work, integrated process design and control of reactive distillation processes that involve multiple elements (more than two) is addressed through a computer-aided hierarchical decomposition-based framework. Multiple elements are encountered for reactive systems when four or more compounds (including inert compounds) are encountered. The reactive distillation design methods and tools which are similar in concept to design of binary non-reactive distillations and binary reactive distillations are used for design of multi-element reactive distillation processes, such as driving force approach. The methods that are used in this work are based on equivalent binary element concept. This concept provides the representation of a multi-element system in terms of two key elements, light key and heavy key elements. First, the reactive distillation column is designed using the equivalent binary element driving force approach. Next, through analytical, steady-state and closed-loop dynamic analysis it is verified that the control structure, disturbance rejection and energy requirement of the reactive distillation column is better than any other operation point that is not at the maximum driving force. Furthermore, it is shown that the design at the maximum driving force can be both controlled using simple controllers such as PI as well as advanced controllers such as MPC.
Reactive distillation, Process design, Process control, Driving force, Computer-aided framework, Multi-element systems
Systematic methods and tools for design of sustainable chemical processes for \( \text{CO}_2 \) utilization

A systematic computer-aided framework for sustainable process design is presented together with its application to the synthesis and generation of processing networks for dimethyl carbonate (DMC) production with \( \text{CO}_2 \) utilization. The framework integrated with various methods, tools, algorithms and databases is based on a combined process synthesis-design-intensification method. The method consists of three stages. The synthesis-stage involves superstructure based optimization to identify promising networks that convert a given set of raw materials to a desired set of products. The design-stage involves selection and analysis of the identified networks as a base case design in terms of operational feasibility, economics, life cycle assessment factors and sustainability measures, which are employed to establish targets for improvement in the next-stage. The innovation-stage involves generation and screening of the more sustainable alternatives through a phenomena-based process intensification method. Applications of the framework are highlighted for the DMC production process.

General information
State: Published
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 2
Systematic screening methodology and energy efficient design of ionic liquid-based separation processes

A systematic methodology for the screening of ionic liquids (ILs) as entrainers and for the design of ILs-based separation processes in various homogeneous binary azeotropic mixtures has been developed. The methodology focuses on the homogeneous binary aqueous azeotropic systems (for example, water+alcohols). Additionally, a Hildebrand solubility parameter group contribution model for ILs, and ILs miscibility database have been developed to screen the miscibility of the ILs with the target solute component and these parameters are considered as the main criteria for the screening of ILs. ILs were further screened based on a combination of criteria such as stability, toxicity, and their environmental impacts. All best ILs were used as entrainers, and an extractive distillation column (EDC) and ionic liquid recovery column were designed and simulated with a process simulator to determine the overall energy consumption of the ILs-based separation processes. Among all candidates, the best IL was selected based on the minimum energy requirement obtained from the simulation. Finally, the modification of the separation process to obtain design flexibility for other azeotropic series with respect to the change in size of the target solute was investigated using the same separation process and IL entrainer to obtain the same product purity. The proposed methodology has been evaluated through a case study of binary alcoholic aqueous azeotropic separation: water+ethanol and water+isopropanol.

General information
State: Published
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Publication: Research - peer-review › Journal article – Annual report year: 2015
System-wide cofactor turnovers can propagate metabolic stability between pathways

Metabolic homeostasis, or low-level metabolic steady state, has long been taken for granted in metabolic engineering, and research priority has always been given to understand metabolic flux control and regulation of the reaction network. In the past, this has not caused concerns because the metabolic networks studied were invariably associated with living cells. Nowadays, there are needs to reconstruct metabolic networks, and so metabolic homeostasis cannot be taken for granted. For metabolic steady state, enzyme feedback control has been known to explain why metabolites in metabolic pathways can avoid accumulation. However, we reasoned that there are further contributing mechanisms. As a new methodology developed, we separated cofactor intermediates (CIs) from non-cofactor intermediates, and identified an appropriate type of open systems for operating putative reaction topologies. Furthermore, we elaborated the criteria to tell if a multi-enzyme over-all reaction path is of in vivo nature or not at the metabolic level. As new findings, we discovered that there are interactions between the enzyme feedback inhibition and the CI turnover, and such interactions may well lead to metabolic homeostasis, an emergent property of the system. To conclude, this work offers a new perspective for understanding the role of CIs and the presence of metabolic homeostasis in the living cell. In perspective, this work might provide clues for constructing non-natural metabolic networks using multi-enzyme reactions or by degenerating metabolic reaction networks from the living cell.

The application of reaction engineering to biocatalysis

Biocatalysis is a growing area of synthetic and process chemistry with the ability to deliver not only improved processes for the synthesis of existing compounds, but also new routes to new compounds. In order to assess the many options and strategies available to an engineer developing a new biocatalytic process, it is essential to carry out a systematic evaluation to progress rapidly and ensure decisions are made on firm foundations. In this way, directed development can be carried out and the chances of implementation of a commercially successful process can be much improved. In this review, we outline the benefits of reaction engineering in this development process, with particular emphasis on reaction kinetics. Future research needs to focus on rapid methods to collect such data at sufficient accuracy that it can be used for the effective design of new biocatalytic processes.
The Current State of Silicone-Based Dielectric Elastomer Transducers

Silicone elastomers are promising materials for dielectric elastomer transducers (DETs) due to their superior properties such as high efficiency, reliability and fast response times. DETs consist of thin elastomer films sandwiched between compliant electrodes, and they constitute an interesting class of transducer due to their inherent lightweight and potentially large strains. For the field to progress towards industrial implementation, a leap in material development is required, specifically targeting longer lifetime and higher energy densities to provide more efficient transduction at lower driving voltages. In this review, the current state of silicone elastomers for DETs is summarised and critically discussed, including commercial elastomers, composites, polymer blends, grafted elastomers and complex network structures. For future developments in the field it is essential that all aspects of the elastomer are taken into account, namely dielectric losses, lifetime and the very often ignored polymer network integrity and stability.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
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Pages: 378-413
Publication date: 2016
Main Research Area: Technical/natural sciences
The effect of cultivation media and washing whole-cell biocatalysts on monoamine oxidase catalyzed oxidative
desymmetrization of 3-azabicyclo[3,3,0]octane

It is well known that washing whole-cells containing enzyme activities after fermentation, but prior to biocatalysis can improve their activity in the subsequent reaction. In this paper, we quantify the impact of both the fermentation media and cell washing on the performance of whole-cell biocatalysis. The results are illustrated using a recombinant monoamine oxidase (expressed in *Escherichia coli*, used in resting state) for the oxidative desymmetrization of 3-azabicyclo[3,3,0]octane. It was shown that the need for washing biocatalyst prior to use in a reaction is dependent upon growth medium. Unlike cells grown in LB medium, washing of the cells was essential for cells grown on TB medium. With TB media, washing the cells improved the final conversion by approximately a factor of two. Additionally, over 50-fold improvement was achieved in initial activity. A potential reason for this improvement in activity was identified to be the increase in transfer of substrates across the cell membrane as a result of cell washing. (C) 2015 Elsevier Inc. All rights reserved.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.83 SJR 0.759 SNIP 1.025
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.061 SNIP 1.214 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.165 SNIP 1.376 CiteScore 3.2
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.204 SNIP 1.281 CiteScore 2.78
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.062 SNIP 1.27 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.201 SNIP 1.565
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.305 SNIP 1.504
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.208 SNIP 1.34
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.976 SNIP 1.257
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.907 SNIP 1.433
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.915 SNIP 1.429
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.847 SNIP 1.263
Scopus rating (2003): SJR 0.798 SNIP 1.218
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.89 SNIP 1.238
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.804 SNIP 1.183
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.668 SNIP 1.191
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.925 SNIP 1.202

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The effect of H$_2$S addition to methane on the ignition and oxidation at high pressures

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, DNV-GL Oil & Gas
Authors: Gersen, S. (Ekstern), van Essen, V. M. (Ekstern), Darmeveil, H. (Ekstern), Hashemi, H. (Intern), Rasmussen, C. L. (Intern), Christensen, J. M. (Intern), Glarborg, P. (Intern), Levinsky, H. B. (Ekstern)
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Electronic versions:
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The Fundamentals Of Bioeconomy The Biobased Society
The population on Earth is growing and we need more food. Climate change is both an actality and a threat. The answer is simple: We absolutely must use our biological resources better, so there will be food for more people with less environmental and climate impact per unit produced, and renewable biological material enough to produce the replacement for what we currently get from fossil crude oil (e.g., materials, chemicals, and plastics).

The good news is that by doing this we can create a lot of new good jobs; and a large part of the technologies are already developed. It is possible. The optimism lies in the fact that in Denmark we are already very good at green technologies, biological production and food production. The next step is to come up in scale, optimize processes and show that it works.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, BioValue SPIR
Authors: Lange, L. (Intern), Lindedam, J. (Ekstern)
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The fundament of food, crop protein production, is threatened by climate change

General information
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The Phase Envelope of Multicomponent Mixtures in the Presence of a Capillary Pressure Difference

Confined fluids such as oil and gas mixtures inside tight reservoirs are systems that can experience high capillary pressure difference between the liquid and gas phases. This capillary pressure difference has an effect on the phase equilibrium and in some cases is considerably high. We presented an algorithm which can reliably compute the whole phase envelope for multicomponent mixtures when there is a capillary pressure difference. It uses an equation of state for the phase equilibrium and the Young-Laplace equation for the capillary pressure model. The algorithm proves to be robust and efficient for test mixtures with wide ranges of compositions at different capillary radii and vapor fractions. The calculation results show that the phase envelope changes everywhere except at the critical point. The bubble point and the lower branch of the dew point show a decrease in the saturation pressure, whereas the upper branch of the dew point shows an increase. The cricondentherm is shifted to a higher temperature. We also presented a mathematical analysis of the phase envelope shift due to capillary pressure based on linear approximations. The resulting linear approximation equations can predict the correct direction of the phase envelope shift. Combined with the multicomponent Clapeyron equation, the equations reveal why the shift changes direction for the saturation pressure at the cricondentherm and for the saturation temperature at the cricondenbar. The equations can be used to estimate the magnitude of shift, and the approximation is close for the change in the bubble point pressure.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
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The Relation Between Structure-Performance of Thin Film Composite Membranes and the Tools Used for Their Fabrication Method

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, University of Southern Denmark, Alfa Laval Automation A/S
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Number of pages: 2
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Source-ID: 2304471835
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Thermodynamic modeling of CO2 mixtures

Knowledge of the thermodynamic properties and phase equilibria of mixtures containing carbon dioxide (CO2) is important in several industrial processes such as enhanced oil recovery, carbon capture and storage, and supercritical extractions, where CO2 is used as a solvent. Despite this importance, accurate predictions of the thermodynamic properties and phase equilibria of mixtures containing CO2 are challenging with classical models such as the Soave-Redlich-Kwong (SRK) equation of state (EoS). This is believed to be due to the fact, that CO2 has a large quadrupole moment which the classical models do not explicitly account for.

In this thesis, in an attempt to obtain a physically more consistent model, the cubic plus association (CPA) EoS is extended to include quadrupolar interactions. The new quadrupolar CPA (qCPA) can be used with the experimental value of the quadrupole moment and with or without introducing an additional pure compound parameter. In the absence of quadrupolar compounds qCPA reduces to CPA, which itself reduces to SRK in the absence of association.

As the number of adjustable parameters in thermodynamic models increase, the parameter estimation problem becomes increasingly complicated due to parameter identifiability issues. In an attempt to quantify and illustrate these issues, the uncertainties in the pure compound parameters of CO2 were investigated using qCPA as well as different CPA approaches. The approaches employ between three and five parameters.

The uncertainties in the parameters were propagated to physical properties, vapor liquid equilibria (VLE), and liquid-liquid equilibria (LLE) using Monte Carlo simulations. The uncertainties in the pure compound parameters were found to be negligible for modeling approaches which employed three adjustable parameters. For modeling approaches with more than three adjustable parameters, however, the uncertainties in the pure compound parameters were significant. As a result the propagated errors were substantial for certain output properties. The uncertainties in VLE were for instance much larger when qCPA was employed with four parameters rather than three. The uncertainty analysis indicated that the parametrization of multi-parameter models is at least as important as the specific model term.

The new qCPA and several CPA approaches were extensively evaluated for their ability to predict the thermodynamic properties of pure CO2. The predictions of these pure compound properties were satisfactory with qCPA, although similar predictions were achieved with the other CPA approaches. The model was subsequently evaluated for its ability to predict and correlate the binary VLE and LLE of mixtures containing CO2 and n-alkanes, water, alcohols, or quadrupolar compounds. For these binary mixtures qCPA appeared to offer systematically improved predictions and correlations as compared to the cases where quadrupolar interactions were ignored. The improvements were particularly pronounced for mixtures of CO2 and hydrocarbons where the model is almost fully predictive.

Finally qCPA was evaluated for its ability to predict the phase equilibria of multicomponent mixtures containing CO2 and n-alkanes, water, and/or alcohols. A single binary interaction parameter was employed in qCPA for most binary combinations. Both qCPA and the best CPA approaches typically performed satisfactorily and predicted the general behavior of the systems, but qCPA used fewer adjustable parameters to achieve similar predictions.

It has been demonstrated that qCPA is a promising model which, compared to CPA, systematically improves the predictions of the experimentally determined phase equilibria between binary and ternary mixtures containing CO2 and other non-quadrupolar compounds. However, for mixtures containing two quadrupolar compounds, or quadrupolar and polar compounds, considerable uncertainty remains as to whether these mixtures are handled in the best possible way. When binary interaction parameters were employed to correlate experimental phase equilibria data, both qCPA and CPA yielded similar correlations - and predictions in the multicomponent case.
thermal) consisting of pure amine vapor pressure, vapor-liquid equilibrium, solid-liquid equilibrium, liquid–liquid equilibrium, excess enthalpy, and heat of absorption of CO₂ in aqueous amine solutions. 94 model parameters and 6 thermodynamic properties were fitted to approximately 1500 experimental data. The developed model accurately represents the equilibrium and thermal data for the studied systems with a single unique set of parameters. The model parameters are valid in the temperature range from −25 to 200 °C, CO₂ partial pressure from 0 to 945 kPa, and concentration of DEEA, MAPA, and CO₂ up to 131, 23, and 33 mol(kg H₂O)⁻¹, respectively. The model calculated speciation are also presented for the studied systems. The model developed in this work can be used for process simulation of CO₂ capture with aqueous blends of DEEA/MAPA.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering  
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**Thermodynamic Property Needs for the Oleochemical Industry**

The oleochemical industry covers mainly the food and pharmaceutical reactions but production of fuels (biodiesel) and other specialty chemical production processes also handle oleochemicals (in other words, lipids). The core of process synthesis and design depend on availability of properties data and/or reliable thermodynamic models for the chemicals involved. Limited availability of consistent physical and thermodynamic properties of lipids compounds and their mixtures lead to difficulties with the use of process simulators for process synthesis and design, since all the models to be used require a priori estimated parameters from experimental data.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre, Alfa Laval Copenhagen A/S
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Texas A and M University at Qatar
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Thermostable β-galactosidases for the synthesis of human milk oligosaccharides

Human milk oligosaccharides (HMOs) designate a unique family of bioactive lactose-based molecules present in human breast milk. Using lactose as a cheap donor, some β-galactosidases (EC 3.2.1.23) can catalyze transgalactosylation to form the human milk oligosaccharide lacto-N-neotetraose (LNnT; Gal-β(1,4)-GlcNAc-β(1,3)-Gal-β(1,4)-Glc). In order to reduce reaction times and be able to work at temperatures, which are less welcoming to microbial growth, the current study investigates the possibility of using thermostable β-galactosidases for synthesis of LNnT and N-acetyllactosamine (LacNAc; Gal-β(1,4)-GlcNAc), the latter being a core structure in HMOs. Two hyperthermostable GH 1 β-galactosidases, Ttβ-gly from Thermus thermophilus HB27 and CelB from Pyrococcus furiosus, were codon-optimized for expression in Escherichia coli along with BgaD-D, a truncated version of the GH 42 β-galactosidase from Bacillus circulans showing high transgalactosylation activity at low substrate concentrations. The three β-galactosidases were compared in the current study in terms of their transgalactosylation activity in the formation of LacNAc and LNnT. In all cases, BgaD-D was the most potent transgalactosidase, but both thermostable GH 1 β-galactosidases could catalyze formation of LNnT and LacNAc, with Ttβ-gly giving higher yields than CelB. The thermal stability of the three β-galactosidases was elucidated and the results were used to optimize the reaction efficiency in the formation of LacNAc, resulting in 5-6 times higher reaction yields and significantly shorter reaction times.
Thiol-ene thermosets exploiting surface reactivity for layer-by-layer structures and control of penetration depth for selective surface reactivity.

Thiol-ene thermosets have been shown to be an efficient platform for preparation of functional polymer surfaces. Especially the effectiveness and versatility of the system has enabled a large variety of network properties to be obtained in a simple and straight-forward way. Due to its selectivity, various thiols and allyl or other vinyl reactants can be used to obtain either soft and flexible or more rigid functional thermosets. The methodology permits use of either thermal or photochemical conditions both for matrix preparation as well as for surface functionalization. Due to excess reactive groups on the surface of thiol-ene thermosets, it is possible to prepare surface functional thermosets or to exploit the reactive groups for modular construction and subsequent chemical bonding. Here a different approach preparing
monolithic layer-by-layer structures with controlled mechanical properties across freestanding samples is presented. The approach is further exploited for preparation of surface structures down to features of 25 μm scale by use of an absorber and simple masking. The combination of masking and absorbers were similarly used to prepare a reactor with controlled surface properties as shown in Figure 1. Here fully sealed reactors (Figure 1a) were prepared modularly by a combination of thiol-ene and thiol-epoxy curing reactions. The reactors were functionalized in different patterns on the top side of the assembled reactor, illustrating the effectiveness of absorbers in controlling the penetration depth and surface grafting. The methodology was used for surface immobilization of enzymes providing a direct link between the distribution of enzymes on the surface and the activity of the reactor.

General information
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Towards an optimal experimental design for N2O model calibration during biological nitrogen removal

Process models describing nitrous oxide (N2O) production during biological nitrogen removal allow for the development of mitigation strategies of this potent greenhouse gas. N2O is an intermediate of nitrogen removal, hence its prediction is negatively affected by the uncertainty associated to its substrates. Improving experimental designs for model calibration reduces prediction uncertainties. Moreover, the individual analysis of autotrophic and heterotrophic contribution to the total NO and N2O pool was assessed for already proposed model structures under different experimental scenarios. The results show the need for information-rich experimental designs to assess the predicting capabilities of N2O models. This work represents a step further in understanding the N2O production and emissions associated to conventional wastewater treatment. Moreover, it will facilitate the development of strategies to minimize the carbon footprint of wastewater treatment plants.

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Toward the Development and Deployment of Large-Scale Carbon Dioxide Capture and Conversion Processes

In light of the depletion of fossil fuels and the increased daily requirements for liquid fuels and chemicals, CO2 should indeed be regarded as a valuable C-1. additional feedstock for sustainable manufacturing of liquid fuels and chemicals. Development and deployment of CO2 capture and chemical conversion processes are among the grand challenges faced by today's scientists and engineers. Very few of the reported CO2 capture and conversion technologies have been employed for industrial installations on a large scale, where high-efficiency, cost/energy-effectiveness, and environmental friendliness are three key factors. The CO2 capture technologies from stationary sources and ambient air based on solvents, solid sorbents, and membranes are discussed first. Transforming CO2 to liquid fuels and chemicals, which are presently produced from petroleum, through thermochemical, electrochemical, photochemical, and biochemical routes are discussed next. The relevant state-of-the-art computational methods and tools as a complement to experiments are also briefly discussed. Finally, after pointing out the advantages and disadvantages of the currently available technologies for CO2 capture and conversion, ideas and perspectives for the development of new techniques, opportunities, and
challenges are highlighted.

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Uncertainty analysis as essential step in the establishment of the dynamic Design Space of primary drying during freeze-drying

Large molecules, such as biopharmaceuticals, are considered the key driver of growth for the pharmaceutical industry. Freeze-drying is the preferred way to stabilise these products when needed. However, it is an expensive, inefficient, time-, and energy-consuming process. During freeze-drying, there are only two main process variables to be set, i.e. the shelf temperature and the chamber pressure, however preferably in a dynamic way. This manuscript focuses on the essential use of uncertainty analysis for the determination and experimental verification of the dynamic primary drying Design Space for pharmaceutical freeze-drying. Traditionally, the chamber pressure and shelf temperature are kept constant during primary drying, leading to less optimal process conditions. In this paper it is demonstrated how a mechanistic model of the primary drying step gives the opportunity to determine the optimal dynamic values for both process variables during processing, resulting in a dynamic Design Space with a well-known risk of failure. This allows running the primary drying process step as time efficient as possible, hereby guaranteeing that the temperature at the sublimation front does not exceed the collapse temperature. The Design Space is the multidimensional combination and interaction of input variables and process parameters leading to the expected product specifications with a controlled (i.e., high) probability. Therefore, inclusion of parameter uncertainty is an essential part in the definition of the Design Space, although it is often neglected. To quantitatively assess the inherent uncertainty on the parameters of the mechanistic model, an uncertainty analysis was performed to establish the borders of the dynamic Design Space, i.e. a time-varying shelf temperature and chamber pressure, associated with a specific risk of failure. A risk of failure acceptance level of 0.01%, i.e. a 'zero-failure' situation, results in an increased primary drying process time compared to the deterministic dynamic Design Space; however, the risk of failure is under control. Experimental verification revealed that only a risk of failure acceptance level of 0.01% yielded a guaranteed zero-defect quality end-product. The computed process settings with a risk of failure acceptance level of 0.01% resulted in a decrease of more than half of the primary drying time in comparison with a regular, conservative cycle with fixed settings. (C) 2016 Published by Elsevier B.V.
Uncertainty analysis of the CPA and a quadrupolar CPA equation of state - With emphasis on CO2

The parameters of thermodynamic models, such as the cubic plus association (CPA) equation of state, are subject to uncertainties due to measurement errors in the experimental data that the models are correlated to. More importantly as the number of adjustable parameters increase, the parameter estimation problem becomes more complicated due to parameter identifiability issues. In this work the uncertainties in the pure compound parameters of CO2 are investigated using several different CPA approaches, including a new quadrupolar CPA. The uncertainties are estimated using both least squares estimation and the bootstrap method for parameter estimation. The uncertainties in the parameters estimated from the bootstrap method are propagated to physical property and vapor liquid equilibrium predictions using
Monte Carlo simulations. The results indicate that both the pure compound parameter uncertainty and the propagated uncertainty are negligible for the modeling approaches which employ three adjustable parameters. For modeling approaches with more than three adjustable parameters, however, there may be significant uncertainties in the pure compound parameters, as well as a high degree of correlation between the adjustable parameters. This results in significant propagated errors for certain output properties. To reduce the uncertainty in the adjustable model parameters the heat of vaporization was included as additional correlation data. This resulted in parameter distributions which followed a normal distribution more closely, however, the correlation between the adjustable parameters remained high. Overall the results indicate that it is important to report parameter uncertainties together with their correlation matrix when a model is developed, so that better informed decisions can be made, for instance about which model extension, or association scheme should be employed.
Upgrading and recovery of fertilizer value of ash from PYRONEER gasification

Low temperature circulating fluidised bed gasifier, alias Pyroneer, allows the production of energy from biomass with high inorganic content like sewage sludge. The use of the resulting Pyroneer ashes in agriculture is important, as they are rich in essential nutrients like P: fertilizer supply is currently dependent on mineral reserves of P, most of which are located outside the European Union. Major concerns are however, the presence of heavy metals and the low plant availability of P in Pyroneer ashes.

Electrodialysis has been studied by other researchers at the Technical University of Denmark as a technique to recover P and remove heavy metals from incineration sewage sludge ashes. In this method, an electrical current is applied to a suspension of ash in an aqueous solution, so as to electromigrate the dissolved ions towards the electrode of opposite polarity. Ion exchange membranes delimitate different compartments and allow the separation of the ionic species, depending on their charge. Thus, P in its neutral to negative forms in solution (H₃PO₄/H₂PO₄⁻/HPO₄²⁻/PO₄³⁻) could be separated from metallic cations, including heavy metals (Cd²⁺, Cu²⁺, etc.). Previous results showed that most P was recovered in an acidic solution depleted of metals, which can potentially be used in the fertilizer industry.

The present PhD study aims to investigate the separation of P from heavy metals in different sewage sludge ashes, with focus on the characteristics deciding P solubility and the development of the suitable electrodialytic method. In total, four ashes produced from three different feedstock were studied:

- One from Pyroneer co-gasification of sewage sludge, in which P was 100% precipitated with phosphate accumulating microorganisms, and wheat straw.
- One from Pyroneer gasification of sewage sludge, in which P was 50% precipitated with Al and Fe salts.
- Two from separate Pyroneer gasification and incineration of the same sewage sludge, the P of which was 30% precipitated with Fe salts.

The results showed that significant amounts of Al/Fe(III)-phosphates could be found through an alkaline leaching in the two ashes from gasification of sewage sludge with chemically precipitated P. In contrast, a considerable lower proportion of Al/Fe(III)-phosphates were found for the incineration sewage sludge ashes, whereas Ca was found to control P solubility at low pH for the ash with biologically precipitated P. Using a 2-compartment electrodialytic cell, in which the ash suspension was acidified, over 80% of P could be recovered from both the Pyroneer ashes with biologically precipitated P and the incineration sewage sludge ashes. However, P recovery was limited to a 40% for the other two ashes using the same setup, which was due to the higher presence of Al/Fe(III)-phosphates. In order to increase the extraction of P for these ashes, an innovative electrodialytic method was designed, for which a patent application was filed. In this new technique, a 2-compartment cell was combined sequentially with a second cell, in which the ash suspension was alkalinised in order to dissolve Al/Fe(III)-phosphates, achieving a recovery of up to 70% of P. The final recovery product in all cases was a diluted H₃PO₄ acid solution (<10 g P/L) with a lower ratio of metallic impurities than in the original ash. Further modifications of the electrodialytic cell allowed a reduction of the ratios of most metals to P to the levels of wet process phosphoric acid, widely used in the manufacturing of fertilizers.
Several other improvements can entail a higher % of P recovery and an optimisation of the electricity consumption. Another membrane technique (forward osmosis) can also increase the concentration of P with minor energy consumption. Nevertheless they need to be addressed in future studies.

**General information**
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**Validation of 3D-CMCC Forest Ecosystem Model (v.5.1) against eddy covariance data for 10 European forest sites**
This study evaluates the performances of the new version (v.5.1) of 3D-CMCC Forest Ecosystem Model (FEM) in simulating gross primary productivity (GPP), against eddy covariance GPP data for 10 FLUXNET forest sites across Europe. A new carbon allocation module, coupled with new both phenological and autotrophic respiration schemes, was implemented in this new daily version. Model ability in reproducing timing and magnitude of daily and monthly GPP fluctuations is validated at intra-annual and inter-annual scale, including extreme anomalous seasons. With the purpose to test the 3D-CMCC FEM applicability over Europe without a site-related calibration, the model has been deliberately parametrized with a single set of species-specific parametrizations for each forest ecosystem. The model consistently reproduces both in timing and in magnitude daily and monthly GPP variability across all sites, with the exception of the two Mediterranean sites. We find that 3D-CMCC FEM tends to better simulate the timing of inter-annual anomalies than their magnitude within measurements’ uncertainty. In six of eight sites where data are available, the model well reproduces the 2003 summer drought event. Finally, for three sites we evaluate whether a more accurate representation of forest structural characteristics (i.e. cohorts, forest layers) and species composition can improve model results. In two of the three sites results reveal that model slightly increases its performances although, statistically speaking, not in a relevant way.

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Organisations: Department of Chemical and Biochemical Engineering, The Euro-Mediterranean Centre for Climate Change, University of Tuscia, University of Exeter, National Research Council of Italy, Free University of Bolzano, University of Antwerp, Dresden University of Technology, Georg-August University Göttingen, Sorbonne Universités, University of Helsinki
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Validation of a plant-wide phosphorus modelling approach with minerals precipitation in a full-scale WWTP

The focus of modelling in wastewater treatment is shifting from single unit to plant-wide scale. Plant wide modelling approaches provide opportunities to study the dynamics and interactions of different transformations in water and sludge streams. Towards developing more general and robust simulation tools applicable to a broad range of wastewater engineering problems, this paper evaluates a plant-wide model built with sub-models from the Benchmark Simulation Model No. 2-P (BSM2-P) with an improved/expended physico-chemical framework (PCF). The PCF includes a simple and validated equilibrium approach describing ion speciation and ion pairing with kinetic multiple minerals precipitation. Model performance is evaluated against data sets from a full-scale wastewater treatment plant, assessing capability to describe water and sludge lines across the treatment process under steady-state operation. With default rate kinetic and stoichiometric parameters, a good general agreement is observed between the full-scale datasets and the simulated results under steady-state conditions. Simulation results show differences between measured and modelled phosphorus as little as 4-15% (relative) throughout the entire plant. Dynamic influent profiles were generated using a calibrated influent generator and were used to study the effect of long-term influent dynamics on plant performance. Model-based analysis shows that minerals precipitation strongly influences composition in the anaerobic digesters, but also impacts on nutrient loading across the entire plant. A forecasted implementation of nutrient recovery by struvite crystallization (model scenario only), reduced the phosphorus content in the treatment plant influent (via centrate recycling) considerably and thus decreased phosphorus in the treated outflow by up to 43%. Overall, the evaluated plant-wide model is able to jointly describe the physico-chemical and biological processes, and is advocated for future use as a tool for design, performance evaluation and optimization of whole wastewater treatment plants. (C) 2016 Elsevier Ltd. All rights reserved.

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Validation of a plant-wide phosphorus modelling approach with minerals precipitation in a full-scale WWTP

The focus of modelling in wastewater treatment is shifting from single unit to plant-wide scale. Plant wide modelling approaches provide opportunities to study the dynamics and interactions of different transformations in water and sludge streams. Towards developing more general and robust simulation tools applicable to a broad range of wastewater engineering problems, this paper evaluates a plant-wide model built with sub-models from the Benchmark Simulation Model No. 2-P (BSM2-P) with an improved/expended physico-chemical framework (PCF). The PCF includes a simple and validated equilibrium approach describing ion speciation and ion pairing with kinetic multiple minerals precipitation. Model performance is evaluated against data sets from a full-scale wastewater treatment plant, assessing capability to describe water and sludge lines across the treatment process under steady-state operation. With default rate kinetic and stoichiometric parameters, a good general agreement is observed between the full-scale datasets and the simulated results under steady-state conditions. Simulation results show differences between measured and modelled phosphorus as little as 4-15% (relative) throughout the entire plant. Dynamic influent profiles were generated using a calibrated influent generator and were used to study the effect of long-term influent dynamics on plant performance. Model-based analysis shows that minerals precipitation strongly influences composition in the anaerobic digesters, but also impacts on nutrient loading across the entire plant. A forecasted implementation of nutrient recovery by struvite crystallization (model scenario only), reduced the phosphorus content in the treatment plant influent (via centrate recycling) considerably and thus decreased phosphorus in the treated outflow by up to 43%. Overall, the evaluated plant-wide model is able to jointly describe the physico-chemical and biological processes, and is advocated for future use as a tool for design, performance evaluation and optimization of whole wastewater treatment plants. (C) 2016 Elsevier Ltd. All rights reserved.

General information
State: Published
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Scopus rating (2012): SJR 2.966 SNIP 2.456 CiteScore 5.15
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.582 SNIP 2.196
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Scopus rating (2009): SJR 2.319 SNIP 2.225
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.065 SNIP 2.19
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.994 SNIP 2.208
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.895 SNIP 2.214
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.114 SNIP 2.337
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.227 SNIP 2.106
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.696 SNIP 1.917
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.54 SNIP 1.775
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.321 SNIP 1.711
Valorization of lignin from biorefineries for fuels and chemicals

Direct lignin liquefaction is a promising process for lignin valorization in which lignin is treated in a solvent at elevated temperature and pressure. Liquefaction of sulfur free lignin obtained as a waste product from 2nd generation bio-ethanol production can provide a sulfur free bio-oil which may substitute fossil fuel. In this Ph.D. study the direct liquefaction of a biorefinery lignin (hydrothermally pretreated enzymatic hydrolysis lignin) is explored. The goal is to provide a bio-crude which can substitute marine diesel as the engines found aboard large ships are adapted to more crude fuels. A novel process, which easily integrates with existing biorefinery infrastructure, is presented. The process yields a lignin-diesel oil (LDO) by noncatalytic solvolysis in ethanol without hydrogen addition. The LDO is superior to pyrolysis oil as it is non-acidic, stable and readily blends with fossil diesel without the need for exhaustive deoxygenation. Batch autoclave experiments on lignin supercritical solvolysis in ethanol revealed the effects of different reaction temperatures, reaction times and degrees of lignin loading on product yields and bio-oil quality. The highest oil yield of 50 wt% dry ash free was obtained for solvolysis of 10 g lignin for 8 h at 400 °C but 47 wt% of the solvent was also disadvantageously consumed. A lower reaction temperature and short reaction time (<1 h) yielded an improved tradeoff between oil yield and solvent consumption. In particular a high lignin:solvent ratio of up to 1:2 (w:w), which is a previously unexplored domain of lignin solvolysis, provided a deoxygenated bio-oil with a low oxygen content of 9.7 wt% and an increasingly narrowed molecular size distribution dominated by species <300 g/mol (lignin monomers and dimers). Decarboxylation is the main contributor to deoxygenation as the majority of CO2 comes from the lignin. Solvent reaction routes were investigated in a separate study where different primary alcohols (methanol, ethanol, 1-propanol and 1-butanol) were used. Primary reactions responsible for solvent loss were direct decomposition to gas through decarbonylation, formation of light condensation products and incorporation of the alcohol into the bio-oil through covalent bonding. The latter may advantageously inhibit repolymerization and improve oil yield. An economic study complemented the results of the parameter study and highlighted that optimum profitability is obtained with short reaction time, high lignin loading and lower reaction temperature such as 350 °C instead of 400 °C. The key challenges of lignin solvolysis in alcohols are optimizing liquefaction fraction yield relative to solvent consumption and continuous processing may provide an improvement.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Nielsen, J. B. (Intern), Jensen, A. D. (Intern), Nielsen, J. (Intern)
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Variation in biochemical composition of Saccharina latissima and Laminaria digitata along an estuarine salinity gradient in inner Danish waters
In European kelp cultivation, knowledge on the spatial variation in biomass productivity and quality needs to be established. The present study provides a detailed overview of the biochemical composition and biomass production potential of Saccharina latissima and Laminaria digitata along a salinity gradient (16–31 PSU) in inner Danish waters. We
discuss the results in a cultivation perspective, and evaluate the potential use of Laminariales as an energy feedstock, a feed additive and a bioremediation tool for mitigating eutrophication. We found the highest biomass production potential, the highest protein content (7.5% of dry matter), and the highest capacity for bio-remediation of nitrogen (1.88% N of dry matter) at high salinities, as opposed to the highest concentrations of fermentable sugars (90% of dry matter) and pigments at low salinities. Thus, areas suitable for high biomass production are not necessarily optimal for producing a specific biomass quality such as high carbohydrate concentration for bioenergy conversion, and this challenges the cultivation practice. Furthermore, concentrations of arsenic in the biomass were generally higher (up to 88 ppm) than allowed for animal diet (40 ppm) and could therefore impose challenges for utilizing S. latissima and L. digitata as animal feed additives.

**General information**

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Scopus rating (2016): CiteScore 4.45 SJR 1.442 SNIP 1.12
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.939 SNIP 1.596 CiteScore 5.53
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Scopus rating (2013): SJR 1.437 SNIP 1.129 CiteScore 4.17
ISI indexed (2013): ISI indexed no
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Source-ID: 2289749237
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**Viden er den vigtigste ingrediens**


**General information**

State: Published
Organisations: Office for Innovation & Sector Services, National Food Institute, Office for Research and Relations, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Research Group for Gut Microbiology and Immunology, Landbrug og Fødevarer, DI Fødevarer, manjourn.dk
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**Publication information**
Visualizing the mobility of silver during catalytic soot oxidation
The catalytic activity and mobility of silver nanoparticles used as catalysts in temperature programmed oxidation of soot:silver (1:5 wt:wt) mixtures have been investigated by means of flow reactor experiments and in situ environmental transmission electron microscopy (ETEM). The carbon oxidation temperature was significantly lower compared to uncatalyzed soot oxidation with soot and silver loosely stirred together (loose contact) and lowered further with the two components crushed together (tight contact). The in situ TEM investigations revealed that the silver particles exhibited significant mobility during the soot oxidation, and this mobility, which increases the soot/catalyst contact, is expected to be an important factor for the lower oxidation temperature. In the intimate tight contact mixture the initial dispersion of the silver particles is greater, and the onset of mobility occurs at a lower temperature which is consistent with the lower oxidation temperature of the tight contact mixture. (C) 2015 Elsevier B.V. All rights reserved.
Water consumption in the energy sector

Energy, water, and food systems are closely interlinked in the Energy-Water-Food Nexus. Water is of paramount importance for the energy sector. Fossil fuels require water for extraction, transport and processing. Thermal power plants require water for cooling, whether they use nuclear, fossil or biofuels. Hydropower is based on water in rivers or reservoirs. Feedstock production for biofuels may depend on water for irrigation. On the other hand, energy is necessary for pumping of ground- and surface water, for water treatment as well as for transport and distribution of water to end-users. The waste water is often returned to the environment after energy requiring waste water management.

General information

State: Published
Organisations: Department of Management Engineering, Systems Analysis, Department of Chemical and Biochemical Engineering, KT Consortium
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Publication date: 2016

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Publisher: Technical University of Denmark (DTU)
Chapter: 5
Main Research Area: Technical/natural sciences
Electronic versions:

DTU INTERNATIONAL_ENERGY_REPORT_2016_reduced.pdf
Publication: Research - peer-review › Report chapter – Annual report year: 2016
Working fluid selection for organic Rankine cycles - Impact of uncertainty of fluid properties
This study presents a generic methodology to select working fluids for ORC (Organic Rankine Cycles) taking into account property uncertainties of the working fluids. A Monte Carlo procedure is described as a tool to propagate the influence of the input uncertainty of the fluid parameters on the ORC model output, and provides the 95%-confidence interval of the net power output with respect to the fluid property uncertainties. The methodology has been applied to a molecular design problem for an ORC using a low-temperature heat source and consisted of the following four parts: 1) formulation of process models and constraints 2) selection of property models, i.e. Peng Robinson equation of state 3) screening of 1965 possible working fluid candidates including identification of optimal process parameters based on Monte Carlo sampling 4) propagating uncertainty of fluid parameters to the ORC net power output. The net power outputs of all the feasible working fluids were ranked including their uncertainties. The method could propagate and quantify the input property uncertainty of the fluid property parameters to the ORC model, giving an additional dimension to the fluid selection process. In the given analysis 15 fluids had an improved performance compared to the base case working fluid.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Mechanical Engineering, Thermal Energy, Technische Universität München
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Scopus rating (2016): CiteScore 5.17 SJR 1.999 SNIP 1.798
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.276 SNIP 2.046 CiteScore 5.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.647 SNIP 2.63 CiteScore 5.7
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.54 SNIP 2.593 CiteScore 5.02
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.998 SNIP 2.25 CiteScore 4.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.609 SNIP 2.043 CiteScore 4
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.814 SNIP 2.725
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.729 SNIP 2.313
Web of Science (2009): Indexed yes
Enhancing SOEC system lifetime by controlling inlet gas composition
In a method for enhancing the lifetime of a solid oxide electrolysis cell system by counteracting nitridation of the threads of the in-line electrical heaters of the system, the start-up, shut-down and trip operations are done in a humidified nitrogen atmosphere on the fuel side to achieve a dew point between -70 DEG C and 23 DEG C, and in air or in carbon dioxide on the oxygen side, securing that sufficiently oxidizing conditions are always present across the whole surface of the cells on the oxygen side in the stack.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Friis Pedersen, C. F. (Ekstern), Bech, L. (Intern), Duhn, J. D. (Intern), Jakobsson, N. B. (Ekstern)
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Rotor for a pyrolysis centrifuge reactor
The present invention relates to a rotor for a pyrolysis centrifuge reactor, said rotor comprising a rotor body having a longitudinal centre axis, and at least one pivotally mounted blade being adapted to pivot around a pivot axis under rotation of the rotor body around the longitudinal centre axis. Moreover, the present invention relates to a pyrolysis centrifuge reactor applying such a rotor.
Scanning rheometer
The present disclosure relates to a filament stretching rheometer for measuring rheological and/or mechanical properties of a sample, comprising: a pair of opposed surfaces for holding the sample therebetween; an actuator configured to provide a controlled axial displacement of at least one of said opposed surfaces; and a sample scanning unit for measuring a diameter of said sample, the sample scanning unit configured for measuring said sample diameter at an axial position controlled independently of the displacement of the opposed surfaces, the sample scanning unit configured for being positioned at a starting point before said controlled axial displacement, wherein the starting point is selected from a position where a minimum diameter of the said sample is determined by said sample scanning unit.

Silicone chain extender
The present invention relates to a silicone chain extender, more particularly a chain extender for silicone polymers and copolymers, to a chain extended silicone polymer or copolymer and to a functionalized chain extended silicone polymer or copolymer, to a method for the preparation thereof and the use thereof.
A 10-day heatwave at flowering superimposed on climate change conditions strongly affects production of 22 barley accessions

Extreme climate events are projected to be among the future most challenging constraints to plant development. Heatwaves as well as floods and droughts cause acute changes in the growth environment determining our primary production (Collins et al., 2013). Europe experienced extreme heatwaves in 2003 and 2006. In 2003, a 21% decrease in the French wheat production was found from temperatures up to 6 °C above long-term means and precipitation being less than 50% of the average (Ciais et al., 2005). One strategy to mitigate the this decrease from heatwaves is to identify resilient cultivars and incorporate them in breeding programs.

In the present study 22 primarily Nordic barley accessions were grown in four basic climate treatments of 1) 19/12°C (day/night) and 400 ppm carbon dioxide concentration [CO₂] mimicking ambient South Scandinavian summer conditions, 2) elevated temperature (+5°C day/night), 3) elevated [CO₂] at 700 ppm and 4) the combination of elevated temperature and [CO₂]. Temperature and [CO₂] were at levels representing a worst case scenario (~RCP8.5, IPCC) at the end of the 21st century. A 10 day-heatwave of 33/22°C (day/night) was superimposed around the time of flowering on the basic climate treatments.

The superimposed heatwave decreased overall grain yield in all combinations, however, vast variation in response was identified among accessions. In the two-factor treatment the decrease in grain yield varied from 2-80%. The heatwave caused the strongest overall effect in the treatment of elevated [CO₂] decreasing grain yield by 48% and the least effect (35%) was observed under elevated temperature suggesting elevated temperature to have a priming effect. In all heatwave treatments allocation of biomass was changed, increasing aboveground vegetative biomass and decreasing grain yield as previously reported.

The treatment with the combination of elevated temperature, [CO₂] and the superimposed heatwave may best represent a future climate scenario since more than one climate factor most likely will change at a time. From the basic ambient treatment to the two-factor treatment including heatwave, grain yield decreased 52%.

Our study emphasizes the need for assessing the effects of extreme events under climate change conditions on numerous accessions in order to select appropriate genotypes for breeding future cultivars that can secure the primary production.
A benchmark simulation model to describe plant-wide phosphorus transformations in WWTPs

It is more than 10 years since the publication of the BSM1 technical report (Copp, 2002). The main objective of BSM1 was to create a platform for benchmarking C and N removal strategies in activated sludge systems. The initial platform evolved into BSM1_LT and BSM2, which allowed for the evaluation of monitoring and plant-wide control strategies, respectively. In addition, researchers working within the IWA Task Group on Benchmarking of Control Strategies for Wastewater Treatment Plants developed other BSM related spin-off products, such as the dynamic influent generator, sensor/actuators/fault models and the different implementations of the ADM1, which have been widely used as standalone applications in both industry and academia. The fact that the BSM platforms (or related material) have resulted in 500+ publications demonstrates (Gernaey et al., 2014) the interest for the tools within the scientific community. In this paper, a highly necessary extension of the BSM2 is proposed. This extension aims at facilitating simultaneous C, N and P removal process development and performance evaluation at a plant-wide level. The main motivation of the work is that numerous wastewater treatment plants (WWTPs) pursue biological/chemical phosphorus removal. However, realistic descriptions of combined C, N and P removal, adds a major, but unavoidable degree of complexity in wastewater treatment process models. This paper identifies and discusses important issues that need to be addressed to upgrade the BSM2 to BSM2-P, for example: 1) new/upgraded mathematical models; 2) model integration; 3) new influent characterization; 4) new plant layout; and, 5) new/extended evaluation criteria. The paper covers and analyses all these aspects at a reasonable level of detail, identifies the main bottlenecks that need to be addressed and presents the simulation results of the first software prototype.

Ab initio and kinetic modeling studies of formic acid oxidation

A detailed chemical kinetic model for oxidation of formic acid (HOCHO) in flames has been developed, based on theoretical work and data from literature. Ab initio calculations were used to obtain rate coefficients for reactions of HOCHO with H, O, and HO2. Modeling predictions with the mechanism have been compared to the experimental results of de Wilde and van Tiggelen (1968) who measured the laminar burning velocities for HOCHO flames over a range of stoichiometries and dilution ratios. The modeling predictions are generally satisfactory. The governing reaction mechanisms are outlined based on calculations with the kinetic model. Formic acid is consumed mainly by reaction with OH, yielding OCHO, which dissociates rapidly to CO2 + H, and HOCO, which may dissociate to CO + OH or CO2 + H, or
react with H, OH, or O2 to form more stable products. The branching fraction of the HOCHO + OH reaction, as well as the fate of HOCO, determines the oxidation rate of formic acid. At lower temperatures HO2, formed from HOCO + O2, is an important chain carrier and modeling predictions become sensitive to the HOCHO + HO2 reaction. © 2014 The Combustion Institute.
Acetate is a superior substrate for microbial fuel cell initiation preceding bioethanol effluent utilization

This study assessed cell voltage development, electricity recovery, and microbial community composition in response to initial substrate including acetate, xylose, acetate/xylose 1:1 mixture (ace/xyl), and bioethanol effluent (BE) during microbial fuel cell (MFC) operation at 1000Ω external resistance. The BE mainly contained 20.5 g/L xylose, 1.8 g/L arabinose, and 2.5 g/L propionic acid. The MFCs initially fed with acetate showed shorter initiation time (1 day), higher average cell voltage (634±9 mV), and higher coulombic efficiency (31.5±0.5 %) than those initially fed with ace/xyl orxylose. However, BE-initiated MFCs only generated 162±1 mV. The acetate-initiated MFCs exhibited longer adaptation time (21 h) and lower cell voltage (645±10 mV) when the substrate was switched to xylose, whereas substrate switching to BE produced the highest voltage (656 mV), maximum power density (362±27 mW/m²), maximum current density (709±27 mA/m²), and coulombic efficiency (25±0.5 %) in the acetate-initiated MFCs. The microbial community in acetate-initiated MFCs was less diverse and contained more electrogenic bacteria (13.9±0.4 %) including Geobacter sulfurreducens and Desulfuromonas acetexigen than the MFCs initially fed with ace/xyl, xylose, and BE. After switching the substrate to xylose and subsequently to BE, the microbial community in the acetate-initiated MFCs became more diverse, while no significant changes were observed in ace/xyl-, xylose-, and BE-initiated MFCs. The results showed that initial substrate affected the power generation and the capability to adapt to the substrate alteration in MFCs. Acetate-initiated MFCs showed best performance in utilizing BE.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Sun, G. (Intern), Thygesen, A. (Intern), Meyer, A. S. (Intern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.254 SNIP 1.217 CiteScore 3.43
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.327 SNIP 1.458 CiteScore 3.71
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.533 SNIP 1.432 CiteScore 4.3
Achieving a More Sustainable Process Design for the Production of Methanol

Methanol is an important chemical product because it can be used as a raw material for the production of other chemicals (1), for example dimethyl carbonate, formaldehyde and methyl tert-butyl ether and it is also one of the most produced bulk chemicals with an annual global production of 100 million metric tonnes per year (1). Methanol can be produced using different reaction paths, for example natural gas. If natural gas is used for methanol production then CO2 is produced, utilized and can be emitted. Therefore, achieving a more sustainable design for the production of methanol is beneficial in order to reduce the process CO2 carbon footprint.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
A comprehensive sensitivity and uncertainty analysis of a milk drying process

A simple steady state model of a milk drying process was built to help process understanding. It involves a spray chamber and also internal/external fluid beds. The model was subjected to a statistical analysis for quality assurance using sensitivity analysis (SA) of inputs/parameters, identifiability analysis (IA) of parameters, and uncertainty analysis (UA) to estimate confidence intervals on parameters and in model predictions. A local method was used for SA, IA was based in the delta mean square and collinearity index calculation, and Maximum Likelihood Estimation was used as the main UA technique. SA results provide evidence towards over-parameterization in the model, and the chamber inlet dry bulb air temperature was the variable (input) with the highest sensitivity. IA results indicated that at most 4 parameters are identifiable: two from spray chamber and one from each fluid bed dryer. Moreover, the confidence intervals obtained for identifiable parameters were reasonable, although two parameters were found significantly correlated. The obtained confidence intervals for model predictions reflect a low uncertainty for the outputs. The rigorously analyzed model is expected to contribute to model-based decision making for process operation and optimization.

Activity and stability of Mo₂C/ZrO₂ as catalyst for hydrodeoxygenation of mixtures of phenol and 1-octanol

Mo₂C/ZrO₂ was investigated as catalyst for hydrodeoxygenation (HDO) of phenol in 1-octanol as a simplified bio-oil model system in a fixed-bed setup at 100bar. Mo₂C/ZrO₂ selectively converted phenol to benzene above 320°C. During long-term testing, limited stability of the catalyst was observed, with the conversion of 1-octanol and phenol decreasing from 70% to 37% and from 37% to 19%, respectively, over 76h of operation. Repeating the experiment but also co-feeding 30% water, the catalyst deactivated completely within 12h of operation. Thermodynamic calculations and in situ XRD analysis showed that Mo₂C is transformed to MoO₂ in the presence of water at the given conditions, and this was probably the source of deactivation in the experiments. Thus, Mo₂C-based catalyst for HDO seems interesting, but requires further stabilization or regeneration of the carbide phase as bio-oil contains high levels of water and water is a by-product during HDO.
Adhesion Strength of Biomass Ash Deposits

This study investigates the shear adhesion strength of biomass ash deposits on superheater tubes. Artificial biomass ash deposits were prepared on superheater tubes and sintered in an oven at temperatures up to 1000°C. Subsequently, the deposits were sheared off with the help of an electrically controlled arm. Higher sintering temperatures resulted in greater adhesion strengths, with a sharp increase observed near the melting point of the ash. Repetition of experiments with fixed operation conditions revealed considerable variation in the obtained adhesion strengths, portraying the stochastic nature of the debonding process.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, DONG Energy A/S
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Number of pages: 6
Publication date: 2015

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Main Research Area: Technical/natural sciences
Conference: The Nordic Flame Days 2015, Copenhagen, Denmark, 06/10/2015 - 06/10/2015
Electronic versions:
Adhesion_Strength_of_Biomass_Ash_Deposits_Yashasvi_Laxminarayan.pdf
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Advanced combustion control for a wood log stove, Expert workshop - Highly Efficient and Clean Wood Log Stoves

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST)
Authors: Illerup, J. B. (Intern), Hansen, B. B. (Intern), Lin, W. (Intern), Nickelsen, J. (Intern), Dam-Johansen, K. (Intern)
Number of pages: 21
Publication date: 2015

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Main Research Area: Technical/natural sciences
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Source-ID: 140786014
Publication: Research › Sound/Visual production (digital) – Annual report year: 2015

A dynamic mathematical model for packed columns in carbon capture plants

In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Carbon capture plants must be operated in synchronization with the operation of thermal power plants. Dynamic and flexible operation of the carbon capture plant is important as thermal plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar in the energy system. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. The dynamic model
developed in this paper is suitable for gas-liquid packed columns, e.g. for CO2 absorption and desorption. The model is based on rigorous thermodynamic and conservation principles and it is set up to preserve these properties upon numerical integration in time. The developed model is applied for CO2 absorption and desorption simulation using monoethanolamine (MEA) and piperazine (PZ) as solvent. MEA is considered as the base-case solvent in the carbon capture business. The effect of changes in the flue gas flow rate and changes in the available steam are investigated to determine their influence on the performance of the capture process. The response of the model is shown in terms of capture efficiency and purity of the CO2 product stream. The model is aimed for rigorous dynamic simulation in the context of optimization and control strategy development.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Gaspar, J. (Intern), Jørgensen, J. B. (Intern), Fosbøl, P. L. (Intern)
Pages: 2738-2743
Publication date: 2015

Aeration control by monitoring the microbiological activity using fuzzy logic diagnosis and control. Application to a complete autotrophic nitrogen removal reactor

Complete Autotrophic Nitrogen Removal (CANR) is a novel process where ammonia is converted to nitrogen gas by different microbial groups. The performance of the process can be compromised by an unbalanced activity of the biomass caused by disturbances or non-optimal operational conditions. This contribution describes the development of a fuzzy-logic based system for both diagnosis and control of a CANR reactor. Based on a combination of measurements of the nitrogen species concentration in the influent and in the effluent on the one hand, and insights into the activities of three distinctive microbial groups on the other hand, the diagnosis provides information on: nitritation, nitratation, anaerobic ammonium oxidation and overall autotrophic nitrogen removal. These four results give insight into the state of the process and are used as inputs for the controller that manipulates the aeration to the reactor. The diagnosis tool was first evaluated using 100 days of real process operation data obtained from a lab-scale single-stage autotrophic nitrogen removing reactor. This evaluation revealed that the fuzzy logic diagnosis is able to provide a realistic description of the microbiological state of the reactor with process engineering insight analysis. An evaluation of both the diagnosis tool and the controller was done by simulating a disturbance in the influent concentration. High and steady nitrogen removal efficiency was achieved thanks to the diagnosis and control system. Finally, development of the diagnosis and control as two independent systems provided further insight into the operation performance, gives transparency towards the operator and makes the system flexible for future maintenance or improvements.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Boiocchi, R. (Intern), Mauricio Iglesias, M. (Intern), Vangsgaard, A. K. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
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A Framework for Modular Modeling of the Diesel Engine Exhaust Gas Cleaning System

Pollutants from diesel engines have a negative effect on urban air quality. Because of this and new legislation restricting the emission level, it is necessary to develop exhaust gas treatment systems for diesel engines that can reduce the amount of pollutants. A modular model capable of simulating the whole catalytic exhaust system would be beneficial towards this goal. A methodology for developing a modular model capable of simulating a system consisting of several sub systems is presented. The methodology describes the steps the user should take to go from problem formulation to the final modular model. Four different models in the automotive diesel exhaust gas cleaning system are presented briefly. Based on the presented methodology, it is discussed which changes are needed to the models to create a modular model of the whole catalytic system.
A Framework for Sustainable Design of Algal Biorefineries: Economic Aspects and Life Cycle Analysis

In this chapter, a framework for sustainable design of algal biorefineries with respect to economic and environmental objectives is presented. As part of the framework, a superstructure is formulated to represent the design space – describing technologies developed for processing various types of algae feedstock for the production of biodiesel and co-products. Relevant data and parameters for each process such as yield, conversion, operational cost is then collected using a standardized format (a generic model) and stored in a database. The sustainable design problem is then formulated mathematically as a mixed integer nonlinear programming problem, and is solved first to identify the optimal designs with respect to economic optimality. These optimal designs are then analyzed further in terms of environmental performance using life cycle analysis. For sustainability analysis, in total five impact categories are calculated including Photochemical oxidation potential (POP), global warming potential (GWP), aquatic ecotoxicity (EcotA), Carcinogenic emissions to urban air (EUAC), and median lethal dose (LD50). To add robustness to the analysis, the framework includes uncertainty analysis using Monte Carlo simulations as well. The application of the framework is highlighted on a case study focusing on feedstock microalgae cultivated in Raceway ponds to produce biodiesel. The framework with the database and superstructure provides an enabling tool to support systematic design and analysis of future and sustainable algal biorefinery concepts.
African perspective on cellulosic ethanol production
A major challenge to commercial production of cellulosic ethanol pertains to the cost-effective breakdown of the complex and recalcitrant structure of lignocellulose into its components via pretreatment, the cost of enzymes for hydrolysis and fermentation, and the conversion rate of C5 sugars to ethanol, among others. While the industrialized and some emerging countries are gradually breaking grounds in cellulosic ethanol, most African countries have made little effort in research and development even though the continent is rich in lignocellulosic biomass. The paper estimates residues from widely available crops and municipal waste and determines their respective theoretical ethanol potential (around 22 billion litres annually). It further reviews stages involved in the production of cellulosic ethanol, focussing on processing methods that can be adapted to current situation in most African countries. The paper suggests that research and development should highlight favourable pretreatment methods such as extrusion, steaming/boiling, and chemical methods employing lime, KOH and crude glycerol (from biodiesel production), as well as the development of crude enzyme complexes from local materials. Though the falling price of enzymes is improving economic production of ethanol, advancements in heterogeneous catalytic hydrolysis will considerably favour economic production of ethanol in Africa due to the potential of recycling and reusing solid acid catalysts.

General information
State: Published
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BFI (2010): BFI-level 1
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A general enhancement factor model for absorption and desorption systems: A CO$_2$ capture case-study

This study derives a general method (GM) for reactive absorption and desorption calculation. It connects the Onda’s approximation for reversible reactions with the van Krevelen’s approach for instantaneous irreversible reactions. It is set-up for a reversible (m+n)-th order, forward reaction kinetics and applied for the CO$_2$-MEA-H$_2$O second order reversible system. The results show that the GM predicts the two-film theory within 2% accuracy and the surface renewal model within 10% accuracy, both at absorber and desorber conditions and for high driving force and pinch conditions. GM is compared to the ideas of van Krevelen, and Astarita and Savage. An analysis demonstrates how the GM model eliminates many of the limitations of previous approaches. It has a noticeable potential to enhance the accuracy of process simulators without sacrificing the simulation time. It could eliminate the need for conservative and uncertain design and therefore it will lead to more realistic cost estimations.
A generalised chemical precipitation modelling approach in wastewater treatment applied to calcite

Process simulation models used across the wastewater industry have inherent limitations due to over-simplistic descriptions of important physico-chemical reactions, especially for mineral solids precipitation. As part of the efforts towards a larger Generalized Physico-chemical Modelling Framework, the present study aims to identify a broadly applicable precipitation modelling approach. The study uses two experimental platforms applied to calcite precipitating from synthetic aqueous solutions to identify and validate the model approach. Firstly, dynamic pH titration tests are performed to define the baseline model approach. Constant Composition Method (CCM) experiments are then used to examine influence of environmental factors on the baseline approach. Results show that the baseline model should include precipitation kinetics (not be quasi-equilibrium), should include a 1st order effect of the mineral particulate state ($X_{\text{cryst}}$) and, for calcite, have a 2nd order dependency (exponent $n = 2.05 \pm 0.29$) on thermodynamic supersaturation ($s$).

Parameter analysis indicated that the model was more tolerant to a fast kinetic coefficient ($k_{\text{cryst}}$) and so, in general, it is
recommended that a large $k_{\text{cryst}}$ value be nominally selected where insufficient process data is available. Zero seed (self nucleating) conditions were effectively represented by including arbitrarily small amounts of mineral phase in the initial conditions. Both of these aspects are important for wastewater modelling, where knowledge of kinetic coefficients is usually not available, and it is typically uncertain which precipitates are actually present. The CCM experiments confirmed the baseline model, particularly the dependency on supersaturation. Temperature was also identified as an influential factor that should be corrected for via an Arrhenius-style correction of $k_{\text{cryst}}$. The influence of magnesium (a common and representative added impurity) on $k_{\text{cryst}}$ was found to be significant but was considered an optional correction because of a lesser influence as compared to that of temperature. Other variables such as ionic strength and pH were adequately captured by the quasi-equilibrium description of the aqueous-phase and no further kinetic corrections were required. The baseline model is readily expandable to include other precipitation reactions. For simple representations, large values for $k_{\text{cryst}}$ with $n \approx 2$ (or $n \approx 2$ or 3 for other minerals, as appropriate) should be selected without corrections to $k_{\text{cryst}}$. Where accuracy is required (e.g., in mechanistic studies), machine estimation of $k_{\text{cryst}}$ should be performed with robust process data and $k_{\text{cryst}}$ should at least be corrected for temperature.

**General information**

State: Published
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BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.319 SNIP 2.225
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A generic methodology for the optimisation of sewer systems using stochastic programming and self-optimizing control

The design of sewer system control is a complex task given the large size of the sewer networks, the transient dynamics of the water flow and the stochastic nature of rainfall. This contribution presents a generic methodology for the design of a self-optimising controller in sewer systems. Such controller is aimed at keeping the system close to the optimal performance, thanks to an optimal selection of controlled variables. The definition of an optimal performance was carried out by a two-stage optimisation (stochastic and deterministic) to take into account both the overflow during the current rain event as well as the expected overflow given the probability of a future rain event. The methodology is successfully applied to design an optimising control strategy for a subcatchment area in Copenhagen. The results are promising and expected to contribute to the advance of the operation and control problem of sewer systems.

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Scopus rating (2016): CiteScore 4.28 SJR 1.141 SNIP 1.779
Waste derived fuels such as Solid Recovered Fuel (SRF) are increasingly being used in the cement industry as a means to reduce cost [1]. SRF is produced by separating the combustible fraction from industrial or municipal solid waste (MSW). The recovered fraction has a higher content of combustible materials such as plastic and paper than mixed MSW [2]. The inhomogeneous nature of SRF [3] makes it difficult to combust and many problems may arise concerning e.g. combustion control, feeding of fuel [2,4], deposit formation [5], or accumulation of impurities [3]. Laboratory ash fusion tests typically show that SRF ash starts melting in the range of 1150-1200 °C [6–8], which is somewhat lower than most coal ashes. However, experiments performed in fluidized bed has shown agglomeration taking place as low as 970-990 °C [9,10], and the predictability by ash fusion tests is generally poor [10]. SRF contains significant quantities of common plastics such as polyethylene (PE), polypropylene (PP), and polyethylene terephthalate (PET). Fluidized bed experiments to examine the pyrolysis of polymers have shown that bed agglomeration can result from melting plastics or sticky char residues in the

**Agglomeration and Deposition Behaviour of Solid Recovered Fuel**

Waste derived fuels such as Solid Recovered Fuel (SRF) are increasingly being used in the cement industry as a means to reduce cost [1]. SRF is produced by separating the combustible fraction from industrial or municipal solid waste (MSW). The recovered fraction has a higher content of combustible materials such as plastic and paper than mixed MSW [2]. The inhomogeneous nature of SRF [3] makes it difficult to combust and many problems may arise concerning e.g. combustion control, feeding of fuel [2,4], deposit formation [5], or accumulation of impurities [3]. Laboratory ash fusion tests typically show that SRF ash starts melting in the range of 1150-1200 °C [6–8], which is somewhat lower than most coal ashes. However, experiments performed in fluidized bed has shown agglomeration taking place as low as 970-990 °C [9,10], and the predictability by ash fusion tests is generally poor [10]. SRF contains significant quantities of common plastics such as polyethylene (PE), polypropylene (PP), and polyethylene terephthalate (PET). Fluidized bed experiments to examine the pyrolysis of polymers have shown that bed agglomeration can result from melting plastics or sticky char residues in the
case of PET [11,12]. The main objective of this study was to characterize the combustion of SRF and especially the deposition propensity of SRF and the main constituents of SRF. This relates both to the low temperature deposits formed during plastic pyrolysis and the high temperature deposits formed by ash. The issues reported in the literature regarding plastic pyrolysis will here be investigated at temperatures above 800 °C that are more common in combustion. It will also be attempted to determine if SRF ash may cause issues below 1000 °C, as indicated by some literature results.

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A high-throughput method for quantifying metabolically active yeast cells
By redesigning the established methylene blue reduction test for bacteria and yeast, we present a cheap and efficient methodology for quantitative physiology of eukaryotic cells applicable for high-throughput systems. Validation of the method in fermenters and high-throughput systems proved equivalent, displaying reduction curves that interrelated directly with CFU counts. For growth rate estimation, the methylene blue reduction test (MBRT) proved superior, since the discriminatory nature of the method allowed for the quantification of metabolically active cells only, excluding dead cells. The drop in metabolic activity associated with the diauxic shift in yeast proved more pronounced for the MBRT-derived curve compared with OD curves, consistent with a dramatic shift in the ratio between live and dead cells at this metabolic event. This method provides a tool with numerous applications, e.g. characterizing the death phase of stationary phase cultures, or in drug screens with pathogenic yeasts.

General information
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One of the major operational challenges experienced by power plants firing biomass is the high corrosion rate of superheaters. This limits the outlet steam temperature of the superheaters and consequently, the efficiency of the power plants. The high corrosion rates have been attributed to the formation of corrosive deposits (rich in alkali chlorides) on the surfaces of the superheaters. Accordingly, an extensive number of fundamental investigations have been undertaken to understand the basic mechanisms behind the alkali chloride induced high temperature corrosion of superheaters (for example, [1–3]). However, complete understanding of the corrosion mechanism under biomass-firing conditions has not yet been achieved. This is attributed partly to the complex nature of the corrosion process since there are many species produced from fuel combustion which can interact with one another and the steel surface. Many studies have focused on specific parameters such as, deposit composition (KCl, K₂SO₄, K₂CO₃, etc.) or gas species such as HCl, SO₂, H₂O [4–6], however, more research is necessary to understand the interaction of deposits and gas mixtures with each other.
and metallic superheater materials.

**General information**

State: Published

Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre

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**A mathematical programming framework for early stage design of wastewater treatment plants**

The increasing number of alternative wastewater treatment technologies and stricter effluent requirements make the optimal treatment process selection for wastewater treatment plant design a complicated problem. This task, defined as wastewater treatment process synthesis, is currently based on expert decisions and previous experiences. This paper proposes a new approach based on mathematical programming to manage the complexity of the problem. The approach generates/identifies novel and optimal wastewater treatment process selection, and the interconnection between unit operations to create a process flow diagram. Towards this end, a superstructure approach is used to represent the treatment alternatives for reaction and separation. A generic process interval model is used to describe each alternative in terms of input/output mass balances including conversion and separation factors. Next the design problem is formulated as a Mixed Integer (Non)linear Programming problem and solved. A case study is formulated and solved to highlight the application of the framework. © 2014 Elsevier Ltd. All rights reserved.

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**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS

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A Method for Sustainable Carbon Dioxide Utilization Process Synthesis and Design

As a result of increasing regulations and concern about the impact of greenhouse gases on the environment, carbon dioxide (CO₂) emissions are a primary focus for reducing emissions and improving global sustainability. One method to achieve reduced emissions, is the conversion of CO₂ to useful compounds via chemical reactions. However, conversion is still in its infancy and requires work for implementation at an industrial level. One aspect of this is the development of a methodology for the formulation and optimization of sustainable conversion processes. This methodology follows three stages for the process synthesis, design and more sustainable design. Using a superstructure-based approach a network of utilization alternatives is created linking CO₂ and other raw materials with various products using processing blocks. This will then be optimized and verified for sustainability. Detailed design has also been performed for various case studies. These case studies include multiple pathways for the production of methanol and the production of dimethyl carbonate (DMC). From detailed design and analysis, CO₂ conversion processes show promise as an additional method for the sustainable reduction of CO₂ emissions.

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A methodological approach to designing sewer system control

When designing sewer system control, there is a lack of methodology and tools that can aid in the design process. In 2004 the PASST1 framework was presented that focuses on determining the potential for control in sewer system operation. However, for the actual design of control systems urban drainage planners still have to rely on their operational knowledge combined with model simulations and trial and error. This is an inefficient process where the final design largely depends on the urban drainage planner’s knowledge about the system dynamics and control in general. The motivation for this thesis was therefore the wish for a methodological approach to sewer system control design. Using a case study the following research hypothesis was tested in this thesis:

Using classical and modern control theory, a methodological approach can be derived for designing sewer system control. This can aid urban drainage planners and other professionals in the planning phase of sewer system control design and effectively contribute to finding novel control solutions.

It was investigated if the established methodology used in classic control theory for process control design can be applied meaningfully to the sewer system. As the methodology takes its basis in a hierarchical decomposition of the control problem based on time-scale, it was also investigated if sewer system control can be decomposed in a similar manner. From a review of existing control systems for sewer systems in Europe, it was concluded that sewer system control can also be decomposed in a hierarchical manner based on differences in time-scale. The proposed time-scale dependent hierarchy for sewer system control contains four layers that each handles their own dedicated task. From the bottom and up they are: 1) the regulatory control layer, 2) the coordinating control layer, 3) the optimisation layer and 4) the management of objectives layer.

The time-scale dependent hierarchy for sewer system control is put into a framework that also contains a terminology related to control. In this way the Planning aid for sewer system real-time control framework can help to compare different control system solutions and facilitate a clear communication between different professions and disciplines working together in sewer system control design.

Starting from the hierarchical decomposition of sewer system control in layers, a stepwise approach to design sewer system control was proposed and followed. The individual layers of the hierarchy were designed one by one for a case study in Copenhagen, with the methods and tools taken from both classical and modern control theory.

The tools of classical control theory are developed for systems that can be approximated by linear models. The main challenge of using classical control theory on the case study was therefore the transient nature and the non-linearity of the sewer system dynamics. The methodology was adapted, by linearizing the sewer system model at various points in time, creating a step-wise linear model. The results of the linearization showed that the sewer system dynamics could be divided into four phases, characterised by the following operation modes: dry weather, filling, saturation, and emptying. Having obtained a piece-wise linear model for each of the operational modes, the tools from classical control theory, such as the calculation of the condition number and the relative gain array, could be successfully applied to the sewer system.

Based on the results, a pairing between the measurements variables and the actuators could be suggested. Having proposed to decompose the sewer system control in a hierarchical manner, it became necessary to investigate the role of the lowest layer in the hierarchy, which is the regulatory control layer. Traditionally the role of the regulatory layer is to reject disturbances and track the setpoints, and the simplest form of regulatory control has just constant setpoints. However, in a transient system like the sewer system, the setpoints may change dramatically and rapidly. Therefore the regulatory control layer may not have the same functionality when designed for the sewer system. From the application of
the classical control theory it was found that the system dynamics could be described by four operational modes, and instead of a fixed setpoint the regulatory control layer needs changing setpoints, according to the operational modes. These can either be fed from a coordinating control layer or from an online optimisation.

To design an optimisation to feed setpoints to the regulatory control layer, modern control theory was applied to the case study. The optimisation was tested when it acted directly on the actuators and when it acted on the regulatory control layer. The two optimisation based control structures were evaluated from a one year simulation and the results showed that there was little difference in the performance. The optimisation based control structures were also compared to the existing control and the regulatory control with set-points coming from the coordinating control layer, and here the latter showed the best performance. This was not unexpected, since the true potential of having optimisation arises, when a system has many control loops with limiting constraints and/or changing prioritisation between them. The results showed that for small sewer systems, where the complexity is limited, it is not necessarily the best option to implement advanced optimisation based control systems. Therefore it is also advisable to approach the design of a control system in a methodological manner, where the design and evaluation can be done step by step.

Based on the experiences gained from designing sewer system control systems for the case study, a systematic methodology for designing sewer system control systems is proposed that combined the steps, control and optimisation tools and methods used throughout the thesis. The proposed methodology provides a basis for gathering experiences with sewer system control design and knowledge sharing; and will help generate control systems of the future that are more robust, more structured, have a better performance and are easier to maintain.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering, Urban Water Engineering
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**A Methodology for a Sustainable CO2 Capture and Utilization Network**
Climate change is a global issue that has come to the forefront of environmental concern. With the increasing emissions of greenhouse gases, efforts have increased to reduce carbon dioxide (CO2) emissions. Regulatory guidelines are becoming more stringent and efforts for long-term reduction are being investigated and implemented [1]. Carbon Capture and Storage (CCS) is the dominant method that is discussed. However, CO2 utilization is receiving increased attention for its ability to help in long-term CO2 reduction and the formation of various chemical products. One of the primary elements of utilization is the conversion of CO2 to valuable products via chemical reactions with other raw materials. In order for this to be implemented at a large and industrial level, further work is necessary. As part of this, the work focuses on the formulation and design of a CO2 utilization network via a superstructure-based methodology.

The method developed involves three stages: a process synthesis stage, a design stage and an innovation stage. Following a superstructure based approach, a network of conversion processes is created. This network links CO2 and products through various processing blocks. Each processing block within the developed network needs to be mathematically described for optimization. The second stage is the detailed design of a path within the network, followed by analysis and improvement by creating a more sustainable design in the innovation stage. An additional element is the sustainable linkage of carbon capture to produce the CO2 feed and the subsequent conversion processes. A manipulation of an MEA absorption process, the current industrial standard for carbon capture [2], is investigated. The resulting CO2 stream can be directly fed into a variety of conversion processes.

However, as not all information is available to describe the network mathematically, the most promising paths based on known technologies are designed and analyzed first. This makes the stages iterative rather than purely sequential. As part of this, a conceptual example of methanol synthesis via CO2 hydrogenation highlights the application. This case study illustrates the utility of the utilization network and elements of the methodology being developed. In addition, the conversion process is linked with carbon capture to evaluate the overall sustainability. Finally, the production of the other raw materials is also analyzed for economic feasibility and environmental sustainability. Using computer-aided methods, the feasibility and sustainability of CO2 conversion is shown through the design and optimization of a methanol synthesis process.

References:
Amine donor and acceptor influence on the thermodynamics of ω-transaminase reactions

In recent years, biocatalytic transamination using ω-transaminase has become established as one of the most interesting routes to synthesize chiral amines with a high enantiomeric purity, especially in the pharmaceutical sector where the demand for such compounds is high. Nevertheless, one limitation for successful implementation and scale-up is that the thermodynamics of such conversions are frequently found unfavourable. Herein, we report experimental measurements of apparent equilibrium constants for several industrially relevant transamination reactions in a systematic manner to better understand the effect of amine acceptor and donor choice. For example, we have found that ortho-substitution of acetophenone like molecules, had a significant impact on the thermodynamic equilibrium. Likewise, the effect of cyclic amine acceptors was evaluated and compared to similar non-cyclic structures. It was found that an aliphatic six-membered ring was favourable and a conjugated bicyclic five-membered ring structure, unfavourable. Finally, we evaluated and compared the use of five different donor molecules, and calculated their ΔGapp values. This is particularly important in the further implementation of such reactions because it may be used to help select suitable donor/acceptor combinations. The results presented here give guidance, with respect to thermodynamics, in order to further extend the application of biocatalytic transamination.
A Model-Based Methodology for Integrated Design and Operation of Reactive Distillation Processes

Process intensification is a new approach that has the potential to improve existing processes as well as new designs of processes to achieve more profitable and sustainable production. However, many issues with respect to their implementation and operation is not clear; for example, the question of operability and controllability. Traditionally process design and process control are considered as independent problems and are solved sequentially. The process design problem is usually solved to achieve the design objectives, and then, the operability and process control issues are identified, analyzed and resolved. A new approach is to tackle process intensification and controllability issues in an integrated manner, in the early stages of process design. This integrated and simultaneous synthesis approach provides optimal operation and more efficient control of complex intensified systems that suffice the process design objectives. Furthermore, it may also suggest innovative process alternatives which are more economical and environmentally sustainable. In this work, a systematic model-based methodology for integrated design and operation of reactive distillation operations is presented. Issues related to operation are addressed to ensure a stable and reliable process design at predefined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions. The methodology employs a decomposition-based method so that the complexity of the problems is reduced into a set of sub-problems that are solved sequentially. The method consists of four hierarchical stages: (1) pre-analysis, (2) steady state analysis, (3) dynamic analysis, and (4) evaluation stage. To illustrate the application of the proposed methodology, production of methyl-tert-butyl-ether (MTBE) using a reactive distillation column (RDC) is considered. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used. The methods are based on the element concept, which is used to translate a ternary system of compounds (methanol, isobutene and MTBE) to a binary system of elements (elements A and B). For a binary element system, a simple reactive McCabe-Thiele-type method (to determine the number of reactive stages) has been used. The reactive equilibrium curve is constructed through sequential calculation of reactive bubble points. For an energy-efficient design, the driving force approach (to determine the optimal feed location) for a reactive system has been employed. For both thereactive McCabe-Thiele and driving force methods, vapor-liquid equilibrium data are based on elements. Thereactive bubble point algorithm is used to compute the reactive vapor-liquid equilibrium data set. The operation of the RDC at the highest driving force and other candidate points is compared through open-loop and closed-loop analysis. By application of this methodology it is shown that designing the process at the maximum driving force results in an energy efficient and operable design. It is verified that the reactive distillation design option is less sensitive to the disturbances in the feed at the highest driving force and has the inherent ability to reject disturbances.
A modern approach for epitope prediction: identification of foot-and-mouth disease virus peptides binding bovine leukocyte antigen (BoLA) class I molecules

Major histocompatibility complex (MHC) class I molecules regulate adaptive immune responses through the presentation of antigenic peptides to CD8+ T cells. Polymorphisms in the peptide binding region of class I molecules determine peptide binding affinity and stability during antigen presentation, and different antigen peptide motifs are associated with specific genetic sequences of class I molecules. Understanding bovine leukocyte antigen (BoLA), peptide-MHC class I binding specificities may facilitate development of vaccines or reagents for quantifying the adaptive immune response to intracellular pathogens, such as foot-and-mouth disease virus (FMDV). Six synthetic BoLA class I (BoLA-I) molecules were produced, and the peptide binding motif was generated for five of the six molecules using a combined approach of positional scanning combinatorial peptide libraries (PSCPLs) and neural network-based predictions (NetMHCpan). The updated NetMHCpan server was used to predict BoLA-I binding peptides within the P1 structural polyprotein sequence of FMDV (strain A24 Cruzeiro) for BoLA-1*01901, BoLA-2*00801, BoLA-2*01201, and BoLA-4*02401. Peptide binding affinity and stability were determined for these BoLA-I molecules using the luminescent oxygen channeling immunoassay (LOCI) and scintillation proximity assay (SPA). The functional diversity of known BoLA alleles was predicted using the MHCcluster tool, and functional predictions for peptide motifs were compared to observed data from this and prior studies. The results of these analyses showed that BoLA alleles cluster into three distinct groups with the potential to define "BoLA supertypes." This streamlined approach identifies potential T cell epitopes from pathogens, such as FMDV, and provides insight into T cell immunity following infection or vaccination.
Analysis and prediction of the alpha-function parameters used in cubic equations of state

The performance of two generalized alpha functions (Soave and generalized Twu functions requiring the acentric factor as input parameter) and two parameterizable alpha functions (Mathias-Copeman and Twu) incorporated in cubic equations of state (Redlich-Kwong and Peng-Robinson) are evaluated and compared regarding their ability to reproduce vapor pressure, heat of vaporization, liquid heat capacity, liquid density and second virial coefficient data. To reach this
objective, extensive databanks of alpha function parameters were created. In particular, pitfalls of Twu-type alpha functions were evidenced and fixed. A new class of purely predictive alpha functions was derived by applying group-contribution (GC) methods to the prediction of alpha function parameters. The interest of such an approach is discussed and compared to another predictive approach (use of generalized alpha functions coupled with GC methods to predict the acentric factor)

**General information**
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Scopus rating (2008): SJR 1.299 SNIP 1.6
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Scopus rating (2007): SJR 1.347 SNIP 1.523
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.308 SNIP 1.553
An electrolyte CPA equation of state for mixed solvent electrolytes

Despite great efforts over the past decades, thermodynamic modeling of electrolytes in mixed solvents is still a challenge today. The existing modeling frameworks based on activity coefficient models are data-driven and require expert knowledge to be parameterized. It has been suggested that the predictive capabilities could be improved through the development of an electrolyte equation of state. In this work, the Cubic Plus Association (CPA) Equation of State is extended to handle mixtures containing electrolytes by including the electrostatic contributions from the Debye-Hückel and Born terms using a self-consistent model for the static permittivity. A simple scheme for parameterization of salts with a limited number of parameters is proposed and model parameters for a range of salts are determined from experimental data of activity and osmotic coefficients as well as freezing point depression. Finally, the model is applied to predict VLE, LLE, and SLE in aqueous salt mixtures as well as in mixed solvents.

General information
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A New Optimization Model for Computer-Aided Molecular Design Problems

Computer-Aided Molecular Design (CAMD) is a method to design molecules with desired properties. That is, through CAMD, it is possible to generate molecules that match a specified set of target properties. CAMD has attracted much attention in recent years due to its ability to design novel as well as known molecules with desired properties. The attention is in particular targeted at the design of chemical based products, such as solvents, refrigerants, active pharmaceutical ingredients, polymers, surfactants, lubricants, and more [1]. Property prediction methods are needed in molecular design, as they enable the prediction of the target properties of the generated candidate molecules from there structural information. Here, CAMD methods can be regarded as the reverse engineering approach to property prediction, as the target properties are known while the molecules that match them need to be determined. In this way, CAMD problems can be formulated as a Mixed Integer Linear/Non-Linear Program (MILP/MINLP). With the advent of
connectivity-based prediction methods, several researchers have developed new strategies for embedding it with CAMD method. Constantinou et al. [2] proposed a systematic strategy for generating isomers from a set of groups. Harper et al. [3] proposed a framework for CAMD method, where the pre-design phase defines the basic needs, the design phase determines the feasible candidates (generates molecules and tests for desired properties) and the post-design phase performs higher level analysis of the molecular structure and the final selection of the product. Samudra and Sahinidis [4] proposed a new optimization model using relaxed property targets and refined property targets with structural corrections. It is usually difficult to model and solve the MILP/MINLP problem with structure information considered due to the increased size of the mathematical problem and number of alternatives. Thus, decomposition-based approach is proposed to solve the problem. In this approach, only first-order groups are considered in the first step to obtain the building block of the designed molecule, then the property model is refined with second-order groups based on the results of the first step. However, this may result in the possibility of an optimal solution being excluded. Samudra and Sahinidis [4] used property relaxation method in the first step to avoid this situation, but it is not always easy for the users to find the appropriate relaxations. On the other hand, the feasible region of the optimization problem will become larger when relaxations are applied, which makes the solution of the problem harder. In this paper, a new model for CAMD problems is proposed. The model has been developed for the consideration of higher order groups in the molecular generation step of CAMD through mathematical optimization [5]. The model can consider both first and second order groups simultaneously in the MILP/MINLP formulation through a set of mathematical constraints. Structural constraints are defined through a set of linear mathematical equations for the feasible generation of molecules and the connectivity of molecular groups through the adjacency matrix. Property constraints are defined from a set of linear constraints based on the group contribution method [2]. The structural information of the molecule is obtained from the solution of the adjacency matrix. The adjacency matrix provides the adjacent connectivity of first order molecular groups. From this, the second order group description is found, which increases the structural information and property prediction accuracy. This will avoid the possible situation in which the optimal point is excluded from the feasible region due to inaccurate property prediction and ensures the obtainability of a global optimal solution. The model is implemented into a GAMS-based environment for the efficient optimization of a given problem. The model applicability will be demonstrated through the solution of a range of product design problems from literature, such as design of simple molecules (solvents and refrigerants) to design of complex molecules (polymers, lipids and surfactants).

General information
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A new soft dielectric silicone elastomer matrix with high mechanical integrity and low losses
Though dielectric elastomers (DEs) have many favourable properties, the issue of high driving voltages limits the commercial viability of the technology. Driving voltage can be lowered by decreasing the Young's modulus and increasing the dielectric permittivity of silicone elastomers. A decrease in Young's modulus, however, is often accompanied by the loss of mechanical stability and thereby the lifetime of the DE. A new soft elastomer matrix, with no loss of mechanical stability and high dielectric permittivity, was prepared through the use of alkyl chloride-functional siloxane copolymers. Furthermore, the increase in dielectric permittivity (43%) was obtained without compromising other important properties of DEs such as viscous and dielectric losses as well as electrical breakdown strength.

General information
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An integrated approach for enhancing biogas yield of manure-based anaerobic digestion

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
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Poster presentation
An Inverse Radiation Model for Optical Determination of Temperature and Species Concentration: Development and Validation

In this study, we present an inverse calculation model based on the Levenberg-Marquardt optimization method to reconstruct temperature and species concentration from measured line-of-sight spectral transmissivity data for homogeneous gaseous media. The high temperature gas property database HITEMP 2010 (Rothman et al. (2010)) contains line-by-line (LBL) information for several combustion gas species, such as CO2 and H2O, was used to predict gas spectral transmissivities. The model was validated by retrieving temperatures and species concentrations from experimental CO2 and H2O transmissivity measurements. Optimal wavenumber ranges for CO2 and H2O transmissivity measured across a wide range of temperatures and concentrations were determined according to the performance of inverse calculations. Results indicate that the inverse radiation model shows good feasibility for measurements of temperature and gas concentration.

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Links: https://aiche.confex.com/aiche/2015/webprogram/Paper436943.html
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A novel control strategy for single-stage autotrophic nitrogen removal in SBR

A novel feedforward–feedback control strategy was developed for complete autotrophic nitrogen removal in a sequencing batch reactor. The aim of the control system was to carry out the regulation of the process while keeping the system close to the optimal operation. The controller was designed based on a process model and then tested experimentally. The resulting batch-to-batch control strategy had the total nitrogen removal efficiency as controlled variable and the setting of the aeration mass flow controller as manipulated variable. Compared to manual operation mode (constant air supply), the controller resulted in a significant performance improvement: removal efficiency was kept at a stable high level in the presence of influent ammonium concentration disturbances, and the absolute deviation on removal efficiency was reduced by 40%. The successful validation of the controller in a lab-scale reactor is a promising result, which brings this control strategy one step closer to full-scale implementation.

General information
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A novel tuning approach for offset-free MPC

Since the beginnings in the chemical and process industry, model based predictive control strategies have become widely accepted. Often mentioned success factors for MPC are the use of optimization based on a plant model, the consideration of constraints, and an intuitive tuning. Indeed, if a nominal plant and overall objective are known, the tuning can become straightforward. However, as soon as disturbances have to be taken into account, the tuning effort increases and becomes less intuitive. Against this background, a novel strategy to address the issues with unknown disturbances is proposed. The idea is to separate the nominal tuning process and extend the control by an outer loop, which ensures offset-free control. The inner, nominal loop decouples the system and essentially leads to a first order response. This inner loop addresses the performance targets in the nominal case, and the outer loop provides offset-free control in case of unknown disturbances. The outer loop consists of feedback controllers adapting the reference, which due to the decoupling can be tuned by known guidelines. The proposed strategy is presented and evaluated using a simulated case study.

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A Numerical Procedure for Model Identifiability Analysis Applied to Enzyme Kinetics

The proper calibration of models describing enzyme kinetics can be quite challenging. In the literature, different procedures are available to calibrate these enzymatic models in an efficient way. However, in most cases the model structure is already decided on prior to the actual calibration exercise, thereby bypassing the challenging task of model structure determination and identification. Parameter identification problems can thus lead to ill-calibrated models with low predictive power and large model uncertainty. Every calibration exercise should therefore be preceded by a proper model structure evaluation by assessing the local identifiability characteristics of the parameters. Moreover, such a procedure should be generic to make sure it can be applied independent from the structure of the model. We hereby apply a numerical identifiability approach which is based on the work of Walter and Pronzato (1997) and which can be easily set up for any type of model. In this paper the proposed approach is applied to the forward reaction rate of the enzyme kinetics proposed by Shin and Kim (1998). Structural identifiability analysis showed that no local structural model problems were occurring. In contrast, the practical identifiability analysis revealed that high values of the forward rate parameter Vf led to identifiability problems. These problems were even more pronounced at higher substrate concentrations, which illustrates the importance of a proper experimental design to avoid (practical) identifiability problems. By using the presented approach it is possible to detect potential identifiability problems and avoid pointless calibration (and
A Perspective on PSE in Fermentation Process Development and Operation

Compared to the chemical industry, the use of PSE methods and tools is not as widespread in industrial fermentation processes. This paper gives an overview of some of the main engineering challenges in industrial fermentation processes. Furthermore, a number of mathematical models are highlighted as examples of PSE methods and tools that are used in the context of industrial fermentation technology. Finally, it is discussed what could be done to increase the future use of PSE methods and tools within the industrial fermentation technology area.

A plant wide aqueous phase chemistry model describing pH variations and ion speciation/pairing in wastewater treatment process models

There is a growing interest within the Wastewater Treatment Plant (WWTP) modelling community to correctly describe physico-chemical processes after many years of mainly focusing on biokinetics (Batstone et al., 2012). Indeed, future modelling needs, such as a plant-wide phosphorus (P) description, require a major, but unavoidable, additional degree of complexity when representing cationic/anionic behaviour in Activated Sludge (AS)/Anaerobic Digestion (AD) systems (Ikumi et al., 2014). In this paper, a plant-wide aqueous phase chemistry module describing pH variations plus ion speciation/pairing is presented and interfaced with industry standard models. The module involves extensive consideration of non-ideality by including ion activities instead of molar concentrations and complex ion pairing. The general equilibria are formulated as a set of Differential Algebraic Equations (DAEs) instead of Ordinary Differential Equations (ODEs) in
order to reduce the overall stiffness of the system, thereby enhancing simulation speed. Additionally, a multi-dimensional version of the Newton-Raphson algorithm is applied to handle the existing multiple algebraic inter-dependencies (Solon et al., 2015). Simulation results show pH predictions when describing Biological Nutrient Removal (BNR) by the activated sludge models (ASM) 1, 2d and 3 (Henze et al., 2000) comparing the performance of a nitrogen removal (WWTP1) and a combined nitrogen and phosphorus removal (WWTP2) treatment plant configuration under different anaerobic/anoxic/aerobic conditions (Flores-Alsina et al., 2012). The same framework is implemented in the Benchmark Simulation Model No. 2 (BSM2) version of the Anaerobic Digestion Model No. 1 (ADM1) (WWTP3) (Batstone et al., 2002; Rosen et al., 2006) as well, predicting pH values at different cationic/anionic loads. In this way, the general applicability/flexibility of the proposed approach is demonstrated by implementing the aqueous phase chemistry module in some of the most frequently used WWTP process simulation models. Finally, it is shown how traditional wastewater modelling studies can be complemented with a rigorous description of aqueous phase and ion chemistry (pH, speciation, complexation).

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A plant-wide aqueous phase chemistry module describing pH variations and ion speciation/pairing in wastewater treatment process models

There is a growing interest within the Wastewater Treatment Plant (WWTP) modelling community to correctly describe physico-chemical processes after many years of mainly focusing on biokinetics. Indeed, future modelling needs, such as a plant-wide phosphorus (P) description, require a major, but unavoidable, additional degree of complexity when representing cationic/anionic behaviour in Activated Sludge (AS)/Anaerobic Digestion (AD) systems. In this paper, a plant-wide aqueous phase chemistry module describing pH variations plus ion speciation/pairing is presented and interfaced with industry standard models. The module accounts for extensive consideration of non-ideality, including ion activities instead of molar concentrations and complex ion pairing. The general equilibria are formulated as a set of Differential Algebraic Equations (DAEs) instead of Ordinary Differential Equations (ODEs) in order to reduce the overall stiffness of the system, thereby enhancing simulation speed. Additionally, a multi-dimensional version of the Newton-Raphson algorithm is applied to handle the existing multiple algebraic inter-dependencies. The latter is reinforced with the Simulated Annealing method to increase the robustness of the solver making the system not so dependant of the initial conditions. Simulation results show pH predictions when describing Biological Nutrient Removal (BNR) by the activated sludge models (ASM) 1, 2d and 3 comparing the performance of a nitrogen removal (WWTP1) and a combined nitrogen and phosphorus removal (WWTP2) treatment plant configuration under different anaerobic/anoxic/aerobic conditions. The same framework is implemented in the Benchmark Simulation Model No. 2 (BSM2) version of the Anaerobic Digestion Model No. 1 (ADM1) (WWTP3) as well, predicting pH values at different cationic/anionic loads. In this way, the general applicability/flexibility of the proposed approach is demonstrated, by implementing the aqueous phase chemistry module in some of the most frequently used WWTP process simulation models. Finally, it is shown how traditional wastewater modelling studies can be complemented with a rigorous description of aqueous phase and ion chemistry (pH, speciation, complexation).

**General information**

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A Posteriori Integration of University CAPE Software Developments
This contribution deals with the mutual integration of existing CAPE software products developed at different universities in Germany, Denmark, and Italy. After the motivation MOSAIC is presented as the bridge building the connection between the modelling tool ICAS-MoT and the numerical processing tool BzzMath. In the main part a case-study is presented, including descriptions of the benefits, challenges, implementation, and application. This paper is completed with aspects of current research activities and a conclusion summarizing the results.

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Application of A Microfluidic Tool for the Determination of Enzyme Kinetics
Biocatalysis offers the ability to carry out important synthesis and production of valuable chemicals at benign conditions. In the development of new processes, enzymes are being engineered towards specific products with great success. Currently, mutations are introduced into enzymes, and mutants are formed thereof and a search among these is conducted. High throughput screening can deliver screening of mutants in the order of millions a day. Enzyme mutants with increased performance are therefore likely to be found. Here, the enzyme amine transaminases is evaluated since it offers a unique way of producing chiral amines. These amines are important as building blocks for pharmaceuticals and agrochemicals. A promising enzyme has been found, but it has been a problem to assess its performance and give process development direction. Common limitations are substrate and product solubility, unfavourable thermodynamics, inhibition and stability. It is a difficult task to assess where the current bottle neck is for a desired process. Moreover, it cannot be expected that a single solution to the limitations can be found and rather an integrated solution of all of the problems should be the future aim. All the limitations surround the reactor of a process, and with the performance of this being unknown, it is almost impossible to direct development. A focal point must therefore lie in the determination of kinetic models and how kinetic data can be obtained in a robust and generic way. Models for many enzymes already exist and can be found in common text books. These models do however require mutant specific data and must be collected with the target reaction. In this thesis a novel way of collecting kinetic data is created, this is carried out by combining existing technology and enables the analysis of aqueous solutions on-line. Furthermore, the use of a size exclusion chromatography column enables the simultaneous detection of enzymes and UV/VIS active compounds. The size exclusion chromatography does not provide baseline separated results, nor is this required. The application of chemometric tools enable detection of compounds in the collected retention time wavelength data. A major improvement over traditional techniques is the quantification of enzyme concentration and this makes it possible to use specific activities for model fitting. The setup takes advantage of microfluidic features and delivers semi-automatic experimentation, overall reducing both consumption of precious materials and costly labor.
Application of CAPEC Lipid Property Databases in the Synthesis and Design of Biorefinery Networks

Petroleum is currently the primary raw material for the production of fuels and chemicals. Consequently, our society is highly dependent on fossil non-renewable resources. However, renewable raw materials are recently receiving increasing interest for the production of chemicals and fuels, so a new industrial system based on biomass, an inexpensive, abundant and renewable raw material, is being established with sustainability as the main driving force [1]. The processing facilities for the production of multiple products (including biofuels and chemicals) from biomass are referred to as biorefineries [2].

The wide variety and complex nature of components in biorefineries pose a challenge with respect to the synthesis and design of these types of processes. Whereas physical and thermodynamic property data or models for petroleum-based processes are widely available, most data and models for biobased processes are not. Lipids are present in biorefinery processes: they represent feedstock (vegetable oil, waste cooking oil, microalgal oil), intermediate products (fatty acids, glycerol) and final products in biorefineries, thus the prediction of their properties is of relevance for the synthesis and design of biorefinery networks.

The objective of this work is to show the application of databases of physical and thermodynamic properties of lipid components to the synthesis and design of biorefinery networks.

Application of Enzyme Coupling Reactions to Shift Thermodynamically Limited Biocatalytic Reactions

In recent years, much interest has been shown in the use of multi-enzyme cascades as a tool in organic synthesis. Such enzymatic cascades can provide added value to a synthetic scheme by starting from cheaper raw materials or making more valuable products. Additionally, they can be used to help shift the equilibrium of otherwise thermodynamically unfavourable reactions to give a higher conversion of the target product. By coupling an energetically unfavourable reaction with a more favourable one, the multi-enzyme cascade mimics the approach taken in nature in metabolic pathways. Nevertheless, it can be challenging to combine several engineered enzymes in vitro for the conversion of non-natural substrates. In this mini-review we focus on enzyme coupling reactions as a tool to alleviate thermodynamic constraints in synthetically useful biocatalytic reactions. The implications of thermodynamic parameters such as the equilibrium constant on the multienzyme cascades and the conventional methods of equilibrium shifting are also discussed in addition to methods used to estimate such values.
Application of microfluidics for the development of intensified aminotransferase (ATA) processes

Development of biocatalytic processes is greatly dominated by well-established batch process based screening technologies, e.g. glass vials (mL) and microtiter plates (μL). However, there is still a need for improvement of currently available technologies and for new technologies enabling relatively easy screening and characterization of different process options. For example, small-scale microfluidic platforms enable testing of complex process options, by combining multiple process steps in a plug-and-play manner, that are difficult to assess with conventional methods. Early in the development of biocatalytic processes, most attention is given to developing and modifying the biocatalyst to reach required process targets. However, it is important to consider the downstream processing (DSP) early in the process development as well, i.e. the downstream costs and limitations to the separation steps will greatly influence the economic viability due to the constraints placed on the required process metrics. This thesis will therefore emphasise product recovery limitations and requirements in combination with the biocatalyst performance and limitations. Here the focus is mainly related to biocatalytic processes where it is found beneficial/necessary to implement in-situ co-product/product removal (IScPR/ISPR). For example, through combined operation of reactor and separation modules, as such applications require selective separation and sufficient driving force to influence the process significantly.

In recent years, many microfluidic applications have proven useful for process and synthesis development within the area of organic synthesis, i.e. flow chemistry. For example, the unique characteristics of the small scale enable safer and efficient handling and production of explosive and/or toxic compounds. Furthermore, development based on applying microfluidic platforms potentially enables easier introduction of continuous process aspects, when suitable. The motivation for this project is to investigate the potential of applying microfluidic technologies in the development and testing of biocatalytic processes. Within this thesis, microfluidic modules are applied as tools to screen, characterize, and test
reactor and separation process options. Furthermore, multiple microfluidic modules are combined in order to test complex process configurations, i.e. reactor modules combined with separation modules, as a means of narrowing down and optimizing the most promising process options.

Throughout this thesis the applicability of microfluidics, as an integrated part of biocatalytic process development, is evaluated based on case studies focusing on the asymmetric synthesis of chiral amines using aminotransferases (ATAs). Chiral amines are valuable building blocks for many pharmaceuticals and precursors. The application of ATAs for asymmetric synthesis has many advantages, but it is also common that there are some challenges. In many cases it is found beneficial/necessary to apply various process engineering strategies, e.g. IScPR and ISPR, to overcome the challenges and ensure the economic feasibility of such processes. With economic process feasibility in mind, it can be extremely useful to apply microfluidic platforms to enable fast screening and characterization of various process options in order to overcome the challenges. Due to the physicochemical properties of the compounds involved in the case studies in this thesis, the focus will be on the application/development of liquid-liquid extraction modules to operate in combination with reactor modules. The main outcome of this PhD thesis is knowledge on the potential of applying microfluidics, in combination with conventional methods, for the development of biocatalytic processes. More specifically, microfluidics will enable testing of complex process options and strategies, which are very difficult to test with conventional methods, by combining microfluidic modules representing different process steps in a plug-and-play manner. The advantages and technology constraining disadvantages of microfluidics for biocatalytic process development are both identified in this thesis. Novel applications of microfluidic development of ATA processes are investigated in detail, i.e. first by characterization of single microfluidic process steps (reactor and liquid-liquid extraction modules) and afterwards by testing of complex processes by combining multiple microfluidic process steps. This is realized by putting in place a microfluidic demonstration system, a plug-and-play combination of a reactor module with two liquid-liquid extraction modules and settlers. Another novelty of this thesis, is the application of the integrated liquid-liquid extraction steps to both recover the product, using in-situ product removal (ISPR), and at the same time feed the main substrate, i.e. in-situ substrate supply (ISSS). Furthermore, guidelines for identifying suitable ISPR/IScPR options – and, importantly, for eliminating unfeasible options – for ATA processes are proposed.

### Application of Multivariate Analysis Tools to Industrial Scale Fermentation Data

The analysis of batch process data can provide insight into the process operation, and there is a vast amount of historical data available for data mining. Empirical modelling utilising this data is desirable where there is a lack of understanding regarding the underlying process (Formenti et al. 2014). This may be the case for fed-batch fermentation processes, where mechanistic modelling is challenging due to non-linear dynamics, and non-steady state operation. There is also a lack of sensors for key parameters which are considered to define the quality of the batch, such as product concentration (Nomikos and MacGregor 1995). Multivariate analysis is a powerful tool for investigating large data sets by identification of trends in the data. However, there are also challenges associated with the application of multivariate analysis tools to batch process data. This is due to issues related to the different batch lengths, different data sampling intervals, noise in the measurements, and both online and offline data. The importance of the pre-processing stages are often underappreciated (Gurden et al. 2001). In this work, a 30 batch dataset from a production process operating at Novozymes A/S is analysed by multivariate analysis with the aim of predicting the final product concentration, which is measured offline at the end of each batch. Many modelling iterations were required using different pre-processing methods, in order to extract the trends from the data set. The final model gave an average prediction error of 7.6%. The success of the final regression model was heavily dependent on the decisions made in the pre-processing stages, where the issues of different batch lengths, different measurement intervals, and variable scaling are considered. Therefore a methodology is presented for future application of multivariate methods to industrial scale process data to cover these considerations.

### General information

**State:** Published  
**Organisations:** Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark, Novozymes A/S, Swiss Federal Institute of Aquatic Science and Technology
Application of New Electrolyte Model to Phase Transfer Catalyst (PTC) Systems

Abstract Phase transfer catalyst (PTC) is used to transfer the desirable active form of an anion from the aqueous phase to organic phase where the reaction occurs. One of major challenges for process design of the PTC system is to establish a reliable thermodynamic model capable of describing phase behaviours of all components including water, organic solvents, inorganic salts, and the PTC. In this work, a new electrolyte model based on the KT-UNIFAC group contribution approach has been developed by adding the Debye-Hückel theory and a second virial coefficient-type term into the KT-UNIFAC model. The temperature-dependent parameters of the new model are introduced to improve the description of phase equilibria in temperature ranges between 273.15 and 373.15 K. The proposed model has been successfully applied to the predictions of phase behaviours of alkali halide aqueous solutions that are usually found in PTC systems, thereby, extending the application range of the PTC-system model. The solubility of PTC in organic solvents, which is a key factor for strategy of PTC and solvent selection, has been calculated using the e-NRTL-SAC model.

A Practical and Fast Method To Predict the Thermodynamic Preference of omega-Transaminase-Based Transformations

A simple, easy-to-use, and fast approach method is proposed and validated that can predict whether a transaminase reaction is thermodynamically unfavourable. This allowed us to de-select, in the present case, at least 50% of the reactions because they were thermodynamically unfavourable as confirmed by experiment. Once a larger data base is established, in silico screening of several new reactions (new target molecules) can easily be performed each day.
A Practical and Fast Method To Predict the Thermodynamic Preference of ω-Transaminase-Based Transformations

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General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, DSM Chemical Technology R&D B.V., DSM Chemtech Center
Authors: Meier, R. J. (Ekstern), Gundersen, M. T. (Intern), Woodley, J. (Intern), Schürmann, M. (Ekstern)
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A Process Concept for High-Purity Production of Amines by Transaminase-Catalyzed Asymmetric Synthesis: Combining Enzyme Cascade and Membrane-Assisted ISPR

For the amine transaminase (ATA)-catalyzed synthesis of chiral amines, the choice of donor substrate is of high importance for reaction and process design. Alanine was investigated as an amine donor for the reductive amination of a poorly water-soluble ketone (4-phenyl-2-butanone) in a combined in situ product removal (ISPR) approach using liquid-membrane extraction together with an enzyme cascade. This ISPR strategy facilitates very high (>98%) product purity with an integrated enrichment step and eliminates product as well as coproduct inhibition. In the presented proof-of-concept alanine shows the following advantages over the other frequently employed amine donor isopropyl amine: (i) nonextractability of alanine affords high product purity without any additional downstream step and no losses via coextraction, (ii) higher maximum reaction rates, and (iii) broader acceptance among ATAs.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University
Authors: Börner, T. (Ekstern), Rehn, G. (Intern), Grey, C. (Ekstern), Adlercreutz, P. (Ekstern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.751 SNIP 1 CiteScore 4.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.88 SNIP 1.102 CiteScore 4.52
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.167 SNIP 1.06 CiteScore 4.82
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.375 SNIP 1.142 CiteScore 4.58
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 2.238 SNIP 1.056 CiteScore 4.3
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 1.664 SNIP 0.926
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A rigorous methodology for development and uncertainty analysis of group contribution based property models

Property prediction models are a fundamental tool of process modeling and analysis, especially at the early stage of process development. Furthermore, property prediction models are the fundamental tool for Computer-aided molecular design used for the development of new refrigerants. Group contribution (GC) based prediction methods use structurally dependent parameters in order to determine the property of pure components. The aim of the GC parameter estimation is to find the best possible set of model parameters that fits the experimental data. In that sense, there is often a lack of attention on numerical and statistical challenges associated with model development and analysis. These challenges include for example (i) performance of optimization algorithms used for finding minimum of the objective function for the parameter estimation, (ii) assessment of parameter estimation errors, (iii) effect of outliers and data pre-treatment, (iv) formulation of parameter estimation problem (e.g. weighted least squares, ordinary least squares, robust regression, etc.) In this study a comprehensive methodology is developed to perform a rigorous and step-by-step assessment and solution of the pitfalls involved in developing models. The methodology takes into account of the following steps.
1) Experimental data collection and providing structural information of molecules. 2) Choice of the regression model: a) ordinary least square b) robust or c) weighted-least-square regression. 
3) Initialization of estimation by use of linear algebra providing a first guess. 
4) Sequential parameter and simultaneous GC parameter by using of 4 different minimization algorithms. 
5) Thorough uncertainty analysis: a) based on asymptotic approximation of parameter covariance matrix b) based on boot strap method. Providing 95%-confidence intervals of parameters and predicted property. 6) Performance statistics analysis and model application. The application of the methodology is shown for a new GC model built to predict lower flammability limit (LFL) for refrigerants. The GC model uses the Marrero-Gani (MR) method which considers the group contribution in different levels both functional and structural. The methodology helps improve accuracy and reliability of property modeling and provides a rigorous model quality check and assurance. This is expected to further their credibility and robustness in wider industrial and scientific applications.

Artificial Neural Networks for Thermochemical Conversion of Biomass

Artificial neural networks (ANNs), extensively used in different fields, have been applied for modeling biomass gasification processes in fluidized bed reactors. Two ANN models are presented, one for circulating fluidized bed gasifiers and another for bubbling fluidized bed gasifiers. Both models determine the producer gas composition and gas yield, using the biomass composition and only a few operating parameters in the input layer. Each model is composed of five ANNs with two neurons in the hidden layer. The backpropagation algorithm is used to train them with published experimental data from other authors. The obtained results show that the percentage composition of the main four gas species in producer gas (CO, CO2, H2, CH4) and producer gas yield for a biomass fluidized bed gasifier, can be successfully predicted by applying neural networks. The results obtained show high agreement with the published experimental data used (R2 > 0.98) and are better than those achieved using a modified thermodynamic equilibrium model. Furthermore, a sensitivity analysis has been applied in each ANN model showing that all selected input variables are important.

A Scientific Basis for the Development of the Next Generation of Biodust Burners

A set of simple kinetic parameters for biomass devolatilization has been derived and validated by tying together experimental setups of different thermal through puts by measurements and CFD simulations. Scaling up combustion processes for qualitative trend assessment all the way from single particle behavior to full-scale industrial application is
A Scientific Basis for the Development of the Next Generation of Biomass Burners

The kinetics derived from the classical engineering study are used to simulate the devolatilization and char burn-out phases in the CFD model. Likewise, the study on morphology development will be used to estimate suitable sub-routines, e.g. effective drag coefficients. The full-scale campaign is used to evaluate the results of the generic CFD models. As the qualitative trends can be reproduced, the CFD models can be used to extend the experimental matrix and facilitate process optimization.

A soft and conductive PDMS-PEG block copolymer as a compliant electrode for dielectric elastomers

Conductive PDMS-PEG block copolymers (Mn = 3 – 5 kg/mol) were chain-extended (Mn = 30 – 45 kg/mol) using hydrosilylation reaction as presented in figure 1. Subsequently, the extended copolymers were added to a conductive nano-filler (multi-walled carbon nanotubes – MWCNTs) in order to enhance conductivity. The combination of soft chainextended PDMS-PEG block copolymers and conductive MWCNTs results in a soft and conductive block copolymer composite which potentially can be used as a compliant and highly stretchable electrode for dielectric elastomers. The addition of MWCNTs into the PDMS-PEG matrix not only increases the conductivity, but also increases mechanical strength by reinforcing the network. However, incorporating MWCNTs into the PDMS-PEG matrix is challenging due to strong van der Waals forces between the MWCNTs. In the present study, MWCNTs were dispersed in organic solvent (N-methyl pyrrolidinone) with 1 wt% of surfactant (Triton X-100). The dispersion of MWCNTs in PDMS-PEG system is shown in figure 2 where MWCNTs are well-distributed in the system indicating an acceptable dispersional though some big clusters appear in the optical microscope image. The conductivity of 4 phr MWCNTs is 10−3 S/cm compared to 10−1 S/cm of a non-stretchable reference conducting silicone elastomer (LR3162 from Wacker). Furthermore, PDMS-PEG block copolymer with 4 phr MWCNTs (Young's modulus, Y = 0.26 MPa) is softer and more stretchable than LR3162 (Y = 1.17 MPa).
A soft and conductive PDMS-PEG block copolymer as a compliant electrode for dielectric elastomers

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: A Razak, A. H. (Intern)
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A solvent evaporation route towards fabrication of hierarchically porous ZSM-11 with highly accessible mesopores
A route to generate hierarchically porous zeolite ZSM-11 has been paved via solvent evaporation induced self-assembly assisted by hexadecyltrimethoxysilane to produce a preformed dry gel, followed by its subsequent transformation into zeolite via steam-assisted-crystallization. The crystallization in dry gel has been found to undergo an orientated attachment growth mechanism whereby hexadecyltrimethoxysilane directs the formation of auxiliary mesopores and inhibits the fusion of primary nucleates. Measurements such as XRD, SEM, TEM, N2-physisorption, and TEM for an inverse replica of Pt derived from hierarchical ZSM-11 have been conducted to characterize the textural properties of the material. Ammonia temperature-programmed-desorption (NH3-TPD) measurements and infrared spectra using probe molecules such as pyridine (Py-IR) and 2,4,6-collidine (Coll-IR) have been collected to investigate the acidic properties as well as the accessibility of the acid sites. The hierarchical ZSM-11 possesses more acid sites on the mesopore surfaces that are accessible towards large probe molecules such as 2,4,6-collidine. This improvement together with the enhanced pore-connectivity brings about an increase in 1,3,5-triisopropylbenzene cracking activity and benzene selectivity with respect to a conventional counterpart.

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, East China University of Science and Technology, Dalian University of Technology
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Web of Science (2017): Indexed yes
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Web of Science (2016): Indexed yes
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Assessment of Recent Process Analytical Technology (PAT) Trends: A Multiauthor Review

This multiauthor review article aims to bring readers up to date with some of the current trends in the field of process analytical technology (PAT) by summarizing each aspect of the subject (sensor development, PAT based process monitoring and control methods) and presenting applications both in industrial laboratories and in manufacture e.g. at GSK, AstraZeneca and Roche. Furthermore, the paper discusses the PAT paradigm from the regulatory science perspective. Given the multidisciplinary nature of PAT, such an endeavour would be almost impossible for a single author, so the concept of a multiauthor review was born. Each section of the multiauthor review has been written by a single expert or group of experts with the aim to report on its own research results. This paper also serves as a comprehensive source of information on PAT topics for the novice reader.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, BASF Schweiz AG, Budapest University of Technology and Economics, ETH Zurich, Bristol-Myers Squibb Company, University of Applied Sciences and Arts Northwestern Switzerland, PharmaCryst Consulting Ltd, Delft University of Technology, GlaxoSmithKline Pharmaceuticals, Hunan University, Newcastle University, Siemens nv/sa, Lappeenranta University of Technology, Roche Ireland Limited, Åbo Academy University, Martin-Luther University, Massachusetts Institute of Technology, Universidade Nova de Lisboa, U.S. Food and Drug Administration, Mettler Toledo AutoChem, FMC Technologies B.V., University of Tulsa, ABB Corporate Research Center, National University of Singapore, Purdue University, Universite Catholique de Louvain, University College Dublin, University of Helsinki
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Scopus rating (2016): CiteScore 2.48 SJR 1.062 SNIP 0.859
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.318 SNIP 1.029 CiteScore 2.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 0.99 CiteScore 2.38
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.13 SNIP 0.977 CiteScore 2.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.185 SNIP 1.12 CiteScore 2.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.212 SNIP 0.914 CiteScore 2.22
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.114 SNIP 0.97
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.046 SNIP 0.922
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.943 SNIP 0.901
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.012 SNIP 0.875
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.083 SNIP 0.882
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.847 SNIP 0.821
Scopus rating (2004): SJR 0.701 SNIP 0.787
Scopus rating (2003): SJR 0.421 SNIP 0.67
Scopus rating (2002): SJR 0.548 SNIP 0.869
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.636 SNIP 0.748
Scopus rating (2000): SJR 0.46 SNIP 0.768
Scopus rating (1999): SJR 0.533 SNIP 0.634

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Research results, Sensor development, Chemical sensors
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A Systematic Computer-Aided Framework for Integrated Design and Control of Chemical Processes

Chemical processes are conventionally designed through a sequential approach. In this sequential approach, first, a steady-state process design is obtained and then, control structure synthesis that, in most of the cases, is based on heuristics is performed. Therefore, process design and process control and operation considerations have been studied independently. Furthermore, this sequential approach does not adequately answer this question, “How process design decisions influence process control and operation?”. In order to answer this question, it is necessary to consider process controllability and operability issues together with process design tasks (Seferlis and Georgiadis, 2004). In this way, it can be assured that design decisions give the optimum operational and economic performance. Operability issues are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions.

In this work, a systematic hierarchical computer-aided framework for integrated process design and control of chemical processes including process intensification is proposed. Note however, because of integration of functions/operations into one system the controllability region of intensified equipment may become smaller (Nikačević et al., 2012). The methodology developed in this work, employs a decomposition-based approach so that the complexity of the problem is reduced into a set of sub-problems that are solved sequentially. The production of methy-tert-butyl-ether (MTBE) is used to demonstrate the application of the framework. First, optimal design-control solution is presented for MTBE production via a reactor-separator-recycle (RSR) system. Next, it will be shown that the RSR system can be replaced by an intensified unit operation, a reactive distillation column (RDC) which optimal design-control solution is also presented. The operation and control of the RSR and RDC at the optimal designs is compared with other candidate designs compared through open-loop and closed-loop analysis. By application of this methodology it is shown that the optimal design obtained from this methodology, it is not only the best from an economic steady-state design point of view, but also from control and operation point view. It is verified that the optimal design options for RSR and RDC are less sensitive to the disturbances in the feed at the optimal design.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana
Authors: Mansouri, S. S. (Intern), Sales-Cruz, M. (Ekstern), Huusom, J. K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
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Event: Abstract from 10th European Congress of Chemical Engineering, Nice, France.
Main Research Area: Technical/natural sciences

A Systematic Modelling Framework for Phase Transfer Catalyst Systems

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana, Korea University
Authors: Anantpinijwatna, A. (Intern), Hyung Kim, S. (Ekstern), Sales-Cruz, M. (Ekstern), Gani, R. (Intern)
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A systematic study of multiple minerals precipitation modelling in wastewater treatment

Mineral solids precipitation is important in wastewater treatment. However approaches to minerals precipitation modelling are varied, often empirical, and mostly focused on single precipitate classes. A common approach, applicable to multi-species precipitates, is needed to integrate into existing wastewater treatment models. The present study systematically tested a semi-mechanistic modelling approach, using various experimental platforms with multiple minerals precipitation.
Experiments included dynamic titration with addition of sodium hydroxide to synthetic wastewater, and aeration to progressively increase pH and induce precipitation in real piggery digestate and sewage sludge digestate. The model approach consisted of an equilibrium part for aqueous phase reactions and a kinetic part for minerals precipitation. The model was fitted to dissolved calcium, magnesium, total inorganic carbon and phosphate. Results indicated that precipitation was dominated by the mineral struvite, forming together with varied and minor amounts of calcium phosphate and calcium carbonate. The model approach was noted to have the advantage of requiring a minimal number of fitted parameters, so the model was readily identifiable. Kinetic rate coefficients, which were statistically fitted, were generally in the range 0.35-11.6 h⁻¹ with confidence intervals of 10-80% relative. Confidence regions for the kinetic rate coefficients were often asymmetric with model-data residuals increasing more gradually with larger coefficient values. This suggests that a large kinetic coefficient could be used when actual measured data is lacking for a particular precipitate-matrix combination. Correlation between the kinetic rate coefficients of different minerals was low, indicating that parameter values for individual minerals could be independently fitted (keeping all other model parameters constant). Implementation was therefore relatively flexible, and would be readily expandable to include other minerals.

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Automated N-glycan profiling of a mutant Trypanosoma rangeli sialidase expressed in Pichia pastoris, using tandem mass spectrometry and bioinformatics

A mutant Trypanosoma rangeli sialidase, Tr7, expressed in Pichia pastoris, exhibits significant trans-sialidase activity, and has been used for analytical-scale production of sialylated human milk oligosaccharides. Mass spectrometry-based site-specific N-glycoprofiling of Tr7 showed that heterogeneous high-mannose type N-glycans were present at all the five potential N-linked glycosites. N-linked glycans in Tr7 were predominantly neutral oligosaccharides with compositions Man₈-16GlcNAc₂, but also mono- and di-phosphorylated oligosaccharides in the forms of Man₉-15P₁GlcNAc₂ and Man₉-14P₂GlcNAc₂, respectively. Some phosphorylated N-linked glycans further contained an additional HexNAc, which has not previously been reported in P. pastoris-expressed proteins. We compiled a method pipeline that combined hydrophilic interaction liquid chromatography enrichment of glycopeptides, high accuracy mass spectrometry and automated interpretation of the mass spectra with in-house developed “MassAI” software, which proved efficient in glycan site microheterogeneity analysis. Functional analysis showed that the deglycosylated Tr7 retained more than 90% of both the sialidase and trans-sialidase activities relative to the glycosylated Tr7.
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Aza-Michael addition reaction: post-polymerization modification and preparation of PEI/PEG-based polyester hydrogels from enzymatically synthesized reactive polymers

The utility of aza-Michael addition chemistry for post-polymerization functionalization of enzymatically prepared polyesters is established. For this, itaconate ester and oligoethylene glycol are selected as monomers. A Candida Antarctica lipase B catalyzed polycondensation reaction between the two monomers provides the polyesters, which carry an activated carbon-carbon double bond in the polymer backbone. These electron deficient alkenes represent suitable aza-Michael acceptors and can be engaged in a nucleophilic addition reaction with small molecular mono-amines (aza-Michael donors) to yield functionalized linear polyesters. Employing a poly-amine as the aza-Michael donor, on the other hand, results in the formation of hydrophilic polymer networks.
Backbone structures in human milk oligosaccharides: trans-glycosylation by metagenomic β-N-acetylhexosaminidases

This paper describes the discovery and characterization of two novel β-N-acetylhexosaminidases HEX1 and HEX2, capable of catalyzing the synthesis of human milk oligosaccharides (HMO) backbone structures with fair yields using chitin oligomers as β-N-acetylglucosamine (GlcNAc) donor. The enzyme-encoding genes were identified by functional screening of a soil-derived metagenomic library. The β-N-acetylhexosaminidases were expressed in Escherichia coli with an N-terminal His6-tag and were purified by nickel affinity chromatography. The sequence similarities of the enzymes with their respective closest homologues are 59% for HEX1 and 51% for HEX2 on the protein level. Both β-N-acetylhexosaminidases were classified into glycosyl hydrolase family 20 (GH 20) and are able to hydrolyze para-nitrophenyl-β-N-acetylglucosamine (pNP-GlcNAc) and para-nitrophenyl-β-N-acetylgalactosamine (pNP-GalNAc) and exhibit pH optima of 8 and 6 for HEX1 and HEX2, respectively. The enzymes are able to hydrolyze N-acetylchitooligosaccharides with a degree of polymerization of two, three, and four. The major findings were, that HEX1 and HEX2 catalyze trans-glycosylation reactions with lactose as acceptor, giving rise to the human milk oligosaccharide precursor lacto-N-tetraose II (LNT2) with yields of 2 and 8% based on the donor substrate. In total, trans-glycosylation reactions were tested with the disaccharide acceptors β-lactose, sucrose, and maltose, as well as with the monosaccharides galactose and glucose resulting in the successful attachment of GlcNAc to the acceptor in all cases. © Springer-Verlag Berlin Heidelberg 2015.
Bilaterally Microstructured Thin Polydimethylsiloxane Film Production

Thin PDMS films with complex microstructures are used in the manufacturing of dielectric electro active polymer (DEAP) actuators, sensors and generators, to protect the metal electrode from large strains and to assure controlled actuation. The current manufacturing process at Danfoss PolyPower A/S produces films with a one-sided microstructured surface only. It would be advantageous to produce a film with both surfaces microstructured, as this increases the film’s performance efficiency. The new technique introduced herein produces bilaterally microstructured film by combining an embossing method with the existing manufacturing process. In employing the new technique, films with microstructures on both surfaces are successfully made with two different liquid silicone rubber (LSR) formulations: 1) pure XLR630 and 2) XLR630 with titanium dioxide (TiO2). The LSR films (~70 μm) are cast on a carrier web substrate using a coating blade. The carrier web, which has a sinusoidal corrugation with wave height of 7μm and a wave period of 7μm on its surface, imparts corrugations to the bottom surface of the film. The elastomer film on the carrier web is preheated to the gel point, where the elastomer film can retain an imprint made on it. The preheated film at gel point is embossed between the rolls of a gravure lab coater, which corrugates the top surface of the film. The films are then heated, in order to cure completely. For the LSR systems used in this process, the optimum conditions for preheating are 110°C for 4–7 s, while for embossing the temperature is 110°C with 25 psi pressure between the rolls at a speed of 1.4 rpm. Scanning electron microscope (SEM) images confirm the formation of microstructures on both the surfaces of the film.
Bio-based alkyds by direct enzymatic bulk polymerization

Alkyd coating systems have been largely used to preserve exterior wood applications as well as to provide them with a decorative appearance. In the current stage of sustainability concerns, there has been a stronger focus on development and production of bio-based coating components, heading toward a totally bio-based formulation. In this context, the biggest challenge is development of bio-based analogues to classical alkyd resins (or alkyd), which is up to 50% fossil based. In addition, all the remaining components of an alkyd coating formulation are also needed to be prepared from renewable raw materials before a 100% bio-based alkyd paint can be realized.

In this project an enzyme catalyzed bulk polymerization method for direct production of alkyds has been developed. The objective has been to make it possible to produce binders at much lower temperatures as well as to achieve a higher degree of control over the polymerization reaction. The process was used to prepare new and 100% bio-based resins. The developed enzymatic method is simple to perform, robust and allows the preparation of alkyds with much higher control over the chemical structure compared with the corresponding traditional method. Bio-based alkyds prepared from a combination of glycerol, and tall oil fatty acids, and azelaic acid by enzymatic polymerization show improved hydrophobicity and lower glass transition temperatures compared to an alkyd prepared from the same raw materials by a classical boiling method. The enzymatic method results in a higher degree of control over the polymerization process, making it possible to optimize the binder structure to a specific degree of branching. Alkyd photostability of glycerol-based alkyds can be improved by increasing the alkyd’s branching level, and subsequent development resulted in optimized structures. It was aimed for further improvement of alkyd photostability through the development of new pentaerythritol-incorporated alkyds with high degree of branching. In order to make it possible to incorporate pentaerythritol into alkyd structures in enzymatic polymerization, a new type of pentaerythritol derivatized with azelaic acid (or penta-aze) was examined and tested for the production of more branched alkyd systems. A photostability test validated the concept, and the method also resulted in alkyds with improved hydrophobicity and lower glass transition temperatures compared to a corresponding classical reference. In a further development of the system, it has been found possible to use the esters of pentaerythritol and stearic acid in combination with the penta-aze derivative for the preparation of pseudo alkyds containing only pentaerythritol as polyol with high degree of branching. Moreover, the studies on more sensitive monomers such as itaconic acid in enzymatic polymerization has showed that the method is useful in the production of alkyds from such building blocks, which could not be prepared by the corresponding classical boiling method at high
temperature. Such systems are considered as a good option for binders with improved curing properties.

In the project various aspects of preparing a bio-based alkyd formulation have also been investigated. In particular, a reaction setup for production of larger amounts of traditional alkyds was designed to allow the production of up to 500 grams of alkyds under inert atmosphere. This system has been used for preparation of a number of bio-based alkyds by classical cooking and provided a selection of physical properties as a function of diacid chain length. The synthesis set up was developed further to enhance reproducibility and emulsification of binders, which ultimately resulted in production of 300 g of a fully biobased alkyd. This binder was efficiently emulsified with a bio-based emulsifier, formulated and subsequently sent to an outdoor exposure, where it will be evaluated over the coming years.

Finally, the project has also been working on the coupling between reinforcement agents and the binder in alkyd coatings. For this purpose, two different types of silica particles were modified with rape seed oil fatty acids or tall oil fatty acids (TOFA-silica), respectively. Tests of TOFA-silica particles have demonstrated that their functionalized surface markedly altered their solubility, but provided only moderate improvement in the mechanical properties of the alkyd.

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**Bioprocess Engineering for the Application of P450s**

Biocatalytic processes are advancing because of their high selectivity and mild operating conditions, in contrast to many chemical catalyzed processes. This is a clear advantage and frequently results in improved environmental performance. Biocatalytic processes have been implemented replacing traditional chemical catalysts as well as enabling new synthesis. Regardless of the process routes, the economic feasibility is crucial for successful industrial implementation. This has also been demonstrated by implemented biocatalytic processes, showing a clear cost advantage compared to the chemical alternative.

One family of enzymes described to have a lot of potential for industrial biocatalysis is cytochrome P450 monooxygenases. The main motivation for this statement is their ability to hydroxylate nonactivated hydrocarbons in a specific manner, using molecular oxygen as oxidant. Containing more than 26 000 enzymes, this family includes diverse enzymes from all kingdoms of life. However, their dependence on cofactor, redox partners and relatively low activity and stability hinders the development of efficient processes. In this thesis, a novel systematic approach has been applied to identify bottlenecks for economically feasible whole cell P450 catalyzed processes to direct research and enable faster implementation. A methodological approach was introduced by reviewing literature based on guidance by economic metrics, followed by cases studies to confirm the initial analysis. The last part of the thesis consists of an economic assessment based on a process model using experimentally gained knowledge, including a sensitivity analysis of the biological parameters protein expression and enzyme total turnover.

Case studies of various complexities have been chosen throughout the thesis. The first case study was performed using a P450 fusion construct expressed in the well explored host Escherichia coli performing ω-hydroxylation of dodecanoic acid. This system represents an artificial fusion construct in a non-natural P450 expressing host. The main limitations in this case were identified to be the stability and activity of the P450, cofactor regeneration by the host cell and substrate inhibition. The latter was partially circumvented by the introduction of substrate in solid form. The second case study utilized a naturally expressing P450 host, Bacillus megaterium, expressing the steroid hydroxylase CYP106A2 for 15β-hydroxylation of cyproterone acetate. The catalytic activity of the overexpressed CYP106A2 was dependent on the natural redox partners in the host cell. The stability of the P450 was also here identified as one of the limitations as well as product inhibition. Product inhibition was in this case addressed by introducing a modified β-cyclodextrin, yielding 98 % conversion in the gram scale.

P450 catalyzed whole cell processes have been identified suitable for production of high value molecules. The main limitations have been shown to be P450 stability and activity, substrate and product inhibition and cofactor regeneration of heterologous expression host. Furthermore, growing cells, where fermentation and biocatalysis is performed in one step is shown to be the most economically feasible option.
Bismuth molybdate catalysts prepared by mild hydrothermal synthesis: Influence of pH on the selective oxidation of propylene

A series of bismuth molybdate catalysts with relatively high surface area was prepared via mild hydrothermal synthesis. Variation of the pH value and Bi/Mo ratio during the synthesis allowed tuning of the crystalline Bi-Mo oxide phases, as determined by X-ray diffraction (XRD) and Raman spectroscopy. The pH value during synthesis had a strong influence on the catalytic performance. Synthesis using a Bi/Mo ratio of 1/1 at pH ≥ 6 resulted in γ-Bi2MoO6, which exhibited a better catalytic performance than phase mixtures obtained at lower pH values. However, a significantly lower catalytic activity was observed at pH = 9 due to the low specific surface area. γ-Bi2MoO6 synthesized with Bi/Mo = 1/1 at pH = 6 and 7 exhibited relatively high surface areas and the best catalytic performance. All samples prepared with Bi/Mo = 1/1, except samples synthesized at pH = 1 and 9, showed better catalytic performance than samples synthesized with Bi/Mo = 2/3 at pH = 4 and 9 and γ-Bi2MoO6 synthesized by co-precipitation at pH = 7. At temperatures above 440 °C, the catalytic activity of the hydrothermally synthesized bismuth molybdates started to decrease due to sintering and loss of surface area. These results support that a combination of the required bismuth molybdate phase and a high specific surface area is crucial for a good performance in the selective oxidation of propylene.
Bridging the Gap between Polymer Melts and Solutions in Extensional Rheology

Since its inception, the tube model of polymer dynamics has undergone several modifications to account for observed experimental trends. One trend that has yet to be captured by a modified version of the tube model is the observed experimental difference between concentrated polymer solutions and polymer melts. We compare the nonlinear extensional rheology of a series of polystyrene solutions with wide concentration range between 10% and 100% (melt) in order to determine the key missing physics that can account for dilution effects. All the solutions studied have the same number of entanglements per chain and are diluted in the same solvent (oligomeric styrene). We show that the difference in nonlinear rheological behavior between polystyrene melts reported by Bach et al.1 and polystyrene solutions reported by Bhattacharjee et al.2 and Sridhar et al.3 can be bridged by changing the polystyrene concentration. The results presented represent a unique benchmark for all future modifications to the tube model.
Brine crude oil interactions at the oil-water interface

The impact of brine salinity and its ionic composition on oil displacement efficiency has been investigated extensively in recent years due to the potential of enhanced oil recovery (EOR). Wettability alterations through relative interactions at the mineral surface have been the basis of proposed mechanisms. The ion specific interaction between fines and polar fractions of crude oil at the oil-water interface has been less explored. In this study the relative affinity between different ions and the oil surface was determined. The experiments prove the importance of Ca\(^{2+}\), SO\(_4^{2-}\), and HPO\(_4^{2-}\) ions in enhancing oil emulsion formation by increasing interactions between polar acids and brine solutions. The results propose the potential use of HPO\(_4^{2-}\) ions in reservoirs having inactive mineral surfaces. The relative oil affinity of different ions including K\(^{+}\), Na\(^{+}\), Mg\(^{2+}\), and Ca\(^{2+}\) (cations), and Cl\(^{-}\), SO\(_4^{2-}\), HPO\(_4^{2-}\), and HCO\(_3^{-}\) (anions), were studied through gas chromatographic analysis. Crude oil from the North Sea was doped with various fractions of organic acids to mimic different polar behavior. Increased brine concentration showed up to 15% upsurge of polar fractions on the oil-water emulsion formation. During emulsion formation the relative interactions at the oil-water interface are proved to follow the Hofmeister series: K\(^{+}\) < Na\(^{+}\) < Mg\(^{2+}\) < Ca\(^{2+}\). Beyond CaCl\(_2\) concentrations of 0.08 mol/l no additional acid participation in emulsion formation was observed. Among anions, SO\(_4^{2-}\) and HPO\(_4^{2-}\) showed optimum emulsion formation at 0.05 mol/l. The amount of emulsion formation showed significant dependency on the type of acid doped in oil. Experiments
demonstrate that the brine solution can alter the micro forces at the oil-water interface, and this ion specific interaction
leads to oil emulsion formation and thus reduces the interfacial viscoelasticity of the trapped oil. These results show
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Calibration and evaluation of predictive accuracy of a (micro)pollutant influent generator
Summary of key findings: The Benchmark Simulation Model No. 2 influent generator upgraded with pharmaceutical
occurrences is capable of reproducing both the long- and short-term dynamics of traditional variables as well as
micropollutants. Several quantitative evaluation criteria are presented and used to assess the model's predictive
capabilities and all show satisfactory results except for COD particulates. Ongoing research aims at improving this
remaining issue.

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Can laccases catalyze bond cleavage in lignin?
Modification of lignin is recognized as an important aspect of the successful refining of lignocellulosic biomass, and
enzyme-assisted processing and upcycling of lignin is receiving significant attention in the literature. Laccases (EC
1.103.2) are taking the centerstage of this attention, since these enzymes may help degrading lignin, using oxygen as the
oxidant. Laccases can catalyze polymerization of lignin, but the question is whether and how laccases can directly
catalyze modification of lignin via catalytic bond cleavage. Via a thorough review of the available literature and detailed
illustrations of the putative laccase catalyzed reactions, including the possible reactions of the reactive radical
intermediates taking place after the initial oxidation of the phenol-hydroxyl groups, we show that i) Laccase activity is able
to catalyze bond cleavage in low molecular weight phenolic lignin model compounds; ii) For laccases to catalyze inter-unit
bond cleavage in lignin substrates, the presence of a mediator system is required. Clearly, the higher the redox potential
of the laccase enzyme, the broader the range of substrates, including o- and p-diphenols, aminophenols, methoxy-
substituted phenols, benzenethiols, polyphenols, and polyamines, which may be oxidized. In addition, the currently
available analytical methods that can be used to detect enzyme catalyzed changes in lignin are summarized, and an
improved nomenclature for unequivocal interpretation of the action of laccases on lignin is proposed. (C) 2015 Elsevier
Inc. All rights reserved.
Cascade catalysis in membranes with enzyme immobilization for multienzymatic conversion of CO$_2$ to methanol

Facile co-immobilization of enzymes is highly desirable for bioconversion methods involving multienzymatic cascade reactions. Here we show for the first time that three enzymes can be immobilized in flat-sheet polymeric membranes simultaneously or separately by simple pressure-driven filtration (i.e. by directing membrane fouling formation), without any addition of organic solvent. Such coimmobilization and sequential immobilization systems were examined for the production of methanol from CO$_2$ with formate dehydrogenase (FDH), formaldehyde dehydrogenase (FaldDH) and alcohol dehydrogenase (ADH). Enzyme activity was fully retained by this non-covalent immobilization strategy. The two immobilization systems had similar catalytic efficiencies because the second reaction (formic acid ! formaldehyde) catalyzed by FaldDH was found to be the cascade bottleneck (a threshold substrate concentration was required). Moreover, the trade-off between the mitigation of product inhibition and low substrate concentration for the adjacent enzymes probably made the coimmobilization meaningless. Thus, sequential immobilization could be used for multi-enzymatic cascade reactions, as it allowed the operational conditions for each single step to be optimized, not only during the enzyme immobilization but also during the reaction process, and the pressure-driven mass transfer (flow-through mode) could overcome the diffusion resistance between enzymes. This study not only offers a green and facile immobilization method for multi-enzymatic cascade systems, but also reveals the reaction bottleneck and provides possible solutions for the bioconversion of CO$_2$ to methanol.

General information

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Cellobiohydrolase and endoglucanase respond differently to surfactants during the hydrolysis of cellulose

Background: Non-ionic surfactants such as polyethylene glycol (PEG) can increase the glucose yield obtained from enzymatic saccharification of lignocellulosic substrates. Various explanations behind this effect include the ability of PEG to increase the stability of the cellulases, decrease non-productive cellulase adsorption to the substrate, and increase the desorption of enzymes from the substrate. Here, using lignin-free model substrates, we propose that PEG also alters the solvent properties, for example, water, leading the cellulases to increase hydrolysis yields.

Results: The effect of PEG differs for the individual cellulases. During hydrolysis of Avicel and PASC with a processive monocomponent exo-cellulase cellobiohydrolase (CBH) I, the presence of PEG leads to an increase in the final glucose concentration, while PEG caused no change in glucose production with a non-processive endoglucanase (EG). Also, no effect of PEG was seen on the activity of beta-glucosidases. While PEG has a small effect on the thermostability of both cellulases, only the activity of CBH I increases with PEG. Using commercial enzyme mixtures, the hydrolysis yields increased with the addition of PEG. In parallel, we observed that the relaxation time of the hydrolysis liquid phase, as measured by LF-NMR, directly correlated with the final glucose yield. PEG was able to boost the glucose production even in highly concentrated solutions of up to 150 g/L of glucose.

Conclusions: The hydrolysis boosting effect of PEG appears to be specific for CBH I. The mechanism could be due to an increase in the apparent activity of the enzyme on the substrate surface. The addition of PEG increases the relaxation time of the liquid-phase water, which from the data presented points towards a mechanism related to PEG-water interactions rather than PEG-protein or PEG-substrate interactions.

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Challenges and opportunities in integration of design and control

Process synthesis and design of plant operation are related topics but current industrial practice solves these problems sequentially. The implication of this sequential strategy may result in design of processing systems which are very hard to control. This paper presents a discussion on drivers for an integrated approach and outlines the challenges in formulation of such a multi-objective synthesis problem. This discussion is viewed in relation to some of the changing trends in the industry. Significant results have been published which in different ways seek to handle the integrated problem. Further,
advancements in control algorithms and software have widened the range of feasible operation and control for strongly interconnected production systems. In light of these advances in different areas of the field, recommendations for further research and initiatives for development of an integrated approach are given with focus on how new results on the short term can improve industrial practice.

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Challenges and opportunities in using Life Cycle Assessment and Cradle to Cradle® for biodegradable bio-based polymers: a review

Both Life Cycle Assessment (LCA) and Cradle to Cradle® (C2C) approaches can provide operative insights in the design of biodegradable bio-based polymers. Some of the challenges shared by both LCA and C2C that need further investigation are the use of lab scale data versus primary data from established technologies and the identification of the best option for the end of use stage, e.g. for use as packaging. We consider the case of a natural fiber-based composite material obtained from barley straw and present some insights from both LCA and C2C perspectives in the identification of the best option for its end of use.

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Challenges encountered calibrating N2O dynamics from mixed cultures

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Characterization and biological depectinization of hemp fibers originating from different stem sections

The wide variation of mechanical properties of natural fibers limits their applications in matrix composites. The aim of this study is to evaluate the properties of hemp fibers from different stem sections (top, middle and bottom) and to assess fungal retting pretreatment of hemp from different stem sections with the white rot fungi Phlebia radiata Cel 26 and Ceriporiopsis subvermispora. For the untreated hemp fibers, no apparent difference in tensile behavior for fiber bundles from different stem sections was observed, and more than 90% tested samples demonstrated plastic flow behavior. Fiber strength and stiffness were highest for the fibers from the top and middle stem sections. These properties were related to the compositional makeup and morphological properties of hemp fibers, notably the secondary fiber cell contents. In fungal retting, there was a strong dependence of depectinization selectivity on stem section, which decreased from bottom to top presumably due to the significantly higher lignin content in the bottom section than in the top section (middle section was in between). Consequently, the fungal retting caused allover reduction in strength of fibers from the bottom section than in those from the top section, and essentially reversed the influence of stem section on fiber tensile strength through depectinization selectivity. At whole hemp stem level, the fungal retting with P. radiata Cel 26 exhibited better mechanical properties with an ultimate tensile strength, strain, and stiffness of 736 MPa, 2.3%, and 42 GPa, respectively, while fibers treated with C. subvermispora exhibited lower mechanical properties of 573 MPa, 1.9%, and 40 GPa, respectively. The study thus also showed that less variable and high strength fibers may be produced using the dependence of depectinization selectivity on stem section for composite application.
Characterization of cellulose fibers by powder diffraction

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Organizations: Department of Chemistry, X-ray Crystallography, Organic Chemistry, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
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**Characterization of the bacterial gut microbiota of piglets suffering from new neonatal porcine diarrhoea**

**Background:** In recent years, new neonatal porcine diarrhoea (NNPD) of unknown aetiology has emerged in Denmark. NNPD affects piglets during the first week of life and results in impaired welfare, decreased weight gain, and in the worst-case scenario death. Commonly used preventative interventions such as vaccination or treatment with antibiotics, have a limited effect on NNPD. Previous studies have investigated the clinical manifestations, histopathology, and to some extent, microbiological findings; however, these studies were either inconclusive or suggested that Enterococci, possibly in interaction with Escherichia coli, contribute to the aetiology of NNPD. This study examined ileal and colonic luminal contents of 50 control piglets and 52 NNPD piglets by means of the qPCR-based Gut Microbiotassay and 16 samples by 454 sequencing to study the composition of the bacterial gut microbiota in relation to NNPD. Results: NNPD was associated with a diminished quantity of bacteria from the phyla Actinobacteria and Firmicutes while genus Enterococcus was more than 24 times more abundant in diarrhoeic piglets. The number of bacteria from the phylum Fusobacteria was also doubled in piglets suffering from diarrhoea. With increasing age, the gut microbiota of NNPD affected piglet and control piglets became more diverse. Independent of diarrhoeic status, piglets from first parity sows (gilts) possessed significantly more bacteria from family Enterobacteriaceae and species E. coli, and fewer bacteria from phylum Firmicutes. Piglets born to gilts had 25 times higher odds of having NNPD compared with piglets born to multiparous sows. Finally, the co-occurrence of genus Enterococcus and species E. coli contributed to the risk of having NNPD. Conclusion: The results of this study support previous findings that points towards genus Enterococcus and species E. coli to be involved in the pathogenesis of NNPD. Moreover, the results indicate that NNPD is associated with a disturbed bacterial composition and larger variation between the diarrhoeic piglets.

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Characterization Scheme for Property Prediction of Fluid Fractions Originating from Biomass

The composition of industrial fluids is often very difficult to identify from the molecular point of view. In the petroleum industry, the use of the so-called “pseudo-components” is commonly accepted in process modeling, and various approaches exist to determine and/or construct them. We have identified and summarized four such approaches, generally based on experimental information such as boiling temperature and density. Fluids that originate from biomass, however, cannot be treated using only volatility, because of the highly polar character and the high molecular weight of its components, resulting in highly nonideal phase equilibrium behavior. In this work, it is proposed to use a more complete set of experimental descriptors in order to determine the chemical structure of an unknown fluid cut. The definition of such a representative molecule (surrogate) makes it possible to use group contribution or other predictive tools for property calculations or characteristic parameters of an equation of state. In order to achieve this goal, a large database of monofunctional molecules (including alcohols, n-aliphatic acids, aldehydes, ketones, aliphatic ethers, esters, n-alkylbenzenes, and alkanes) has been constructed, which contains a number of descriptors originating from analytical measurements. Using physical insight on the molecular interactions, an algorithm is proposed that uses five descriptors (molecular weight, liquid molar volume, viscosity, refractive index, and dielectric constant) in order to reconstruct a representative molecule.

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Climate effect of an integrated wheat production and bioenergy system with Low Temperature Circulating Fluidized Bed gasifier

When removing biomass residues from the agriculture for bioenergy utilization, the nutrients and carbon stored within these "residual resources" are removed as well. To mitigate these issues the energy industry must try to conserve and not destroy the nutrients. The paper analyses a novel integration between the agricultural system and the energy system through the Low Temperature Circulating Fluidized Bed (LT-CFB) gasifier from the perspective of wheat grain production and electricity generation using wheat straw, where the effects of removing the straw from the agricultural system are assessed along with the effects of recycling the nutrients and carbon back to the agricultural system. The methods used to assess the integration was Life Cycle Assessment (LCA) with IPCC's 2013 100 year global warming potential (GWP) as impact assessment method. The boundary was set from cradle to gate with two different functional units, kg grain and kWh electricity produced in Zealand, Denmark. Two cases were used in the analysis: 1. nutrient balances are regulated by mineral fertilization and 2. the nutrient balances are regulated by yield. The analysis compare three scenarios of gasifier operation based on carbon conversion to two references, no straw removal and straw combustion. The results show that...
the climate effect of removing the straws are mitigated by the carbon soil sequestration with biochar, and electricity and district heat substitution. Maximum biochar production outperforms maximum heat and power generation for most substituted electricity and district heating scenarios. Irrespective of the substituted technologies, the carbon conversion needs to be 80-86% to fully mitigate the effects of removing the straws from the agricultural system. This concludes that compromising on energy efficiency for biochar production can be beneficial in terms of climate change effect of an integrated wheat production and bioenergy system.
Combustion Characterization of Bio-derived Fuels and Additives

Climate change has become a serious concern nowadays. The main reason is believed to be the high emission of greenhouse gases, namely CO2 which is mainly produced from the combustion of fossil fuels. At the same time, energy demand has increased exponentially while the energy supply mainly depends on fossil fuels, especially for transportation. The practical strategy to address such problems in medium term is to increase the efficiency of combustion-propelled energy-production systems, as well as to reduce the net release of CO2 and other harmful pollutants, likely by using nonconventional fuels. Modern internal combustion engines such as Homogeneous Charge Compression Ignition (HCCI) engines are more efficient and fuel-flexible compared to the conventional engines, making opportunities to reduce the release of greenhouse and other polluting gases to the environment. Combustion temperature in modern engines, gas turbines, and industrial burners has been reduced to prevent nitrogen oxides (NOx) formation. Besides that, the pressure has commonly been elevated to promote the efficiency of the systems. Under such conditions, ignition and pollutant formation are determined by reaction kinetic. Alternative fuels may be produced from different sources. If biomass feedstock is used in their production, they have the potential to reduce the net CO2 release to the environment. However, the oxidation chemistry of alternative fuels is less known compared to the conventional fuels. In design/optimization of modern combustion-propelled systems reliable chemical kinetic models are vital while such models are rare for alternative fuels. This knowledge gap has been a challenging factor in utilizing alternative fuels in large scale. This thesis is dedicated to provide characteristic data for fuel oxidation at high pressure and intermediate temperature. Such data provide a detailed insight into the oxidation chemistry and are vital tools in developing chemical kinetic models. Selected iii fuels for this study, hydrogen, methane, ethane, ethanol, and dimethyl ether (DME), all can be produced from bio-sources. Their reaction kinetics are essential in modeling more complicated bio-derived fuels. Moreover, hydrogen, ethanol, and DME have been considered as additives to improve combustion properties of other fuels. In this work, experiments were carried out in a laminar flow reactor at the temperatures of 450– 900 K and pressures of 20–100 bar. The results provided information about the onset temperature of reaction and the gas composition upon reaction initiation. A wide range of stoichiometry was tested, from very fuel-lean to strong fuel-rich mixtures. For ethanol and DME, further pyrolysis experiments were carried out. The results indicated that the onset temperature of reaction varied considerably among the fuels. DME highly diluted in nitrogen ignited at 525 K, independent of the stoichiometry and much lower compared to the other fuels. Ethane, ethanol, methane, and hydrogen ignited at higher temperatures, subsequently. The effect of doping methane by DME was also investigated and it was found that even small amount of DME can promote the methane oxidation considerably. The flow reactor data have been interpreted in terms of a detailed chemical kinetic model, drawn mostly from earlier work from the same laboratory. The modeling predictions have been in good agreement with the measurements in the flow reactor. The model was further evaluated against high-pressure ignition delays as well as flame speed measurements in literature, and it successfully predicted most of the data. The reaction pathway of different fuels have been discussed, and sensitive reactions have been identified. A few reactions with high sensitivity but with poorly determined rate constants have been identified for further studies. The model was also used to analyze the complex behavior of the ignition of selected fuels against temperature and pressure. This mechanism can be utilized for further studies involving oxidation at high pressures and intermediate temperatures.
Combustion Characterization of Individual Bio-oil Droplets

Single droplet combustion characteristics have been investigated for bio-oil slurries, containing biomass residue, and compared to conventional fuels for pulverized burners, such as fuel oil (start up) and wood chips (solid biomass fuel). The investigated fuels ignition delays and pyrolysis behavior was tested in a single particle reactor at conditions relevant for suspension firing (A: 1200 °C, 5.5 % O2; B: 1200 °C, 2.9 % O2 and C: 990 °C, 5.5 % O2). The slurries were tested to optimize the bio-oil composition for use as an alternative power plant start-up fuel. Pyrolysis times for 5 mg bio-oil samples (app. dp 1 mm) were generally in a similar range (1300 to 2700 ms) as fuel oil, (app 1800 ms) and wood blocks (app 2400 ms), within the 600 ms standard deviation. The 5 different bio-oil slurries samples showed considerable data variability, indicating some extent of sample heterogeneity. With respect to the ignition delay, the bio-oils were in contrast to the fuel oil (125±70 ms), associated with either a longer ignition delay or an ignition phase with sporadic gas phase ignitions (350 to 1050 ms with no stable flame), which could be a cause for concern for a start-up fuel, due to flame lift above the nozzles and thereby decreased flame stability. Most promising were oil or diesel (not palm oil) containing slurries (1 and 5) with heating values in the range of 15 MJ/kg.

Comparison of Different Pretreatment Strategies for Ethanol Production of West African Biomass

Pretreating lignocellulosic biomass for cellulosic ethanol production in a West African setting requires smaller scale and less capital expenditure compared to current state of the art. In the present study, three low-tech methods applicable for West African conditions, namely Boiling Pretreatment (BP), Soaking in Aqueous Ammonia (SAA) and White Rot Fungi pretreatment (WRF), were compared to the high-tech solution of hydrothermal pretreatment (HTT). The pretreatment methods were tested on 11 West African biomasses, i.e. cassava stalks, plantain peelings, plantain trunks, plantain leaves, cocoa husks, cocoa pods, maize cobs, maize stalks, rice straw, groundnut straw and oil palm empty fruit bunches. It was found that four biomasses’ (plantain peelings, plantain trunks, maize cobs and maize stalks) were most promising for production of cellulosic ethanol with profitable enzymatic conversion of glucan (>30 g glucan per 100 g total solids (TS)). HTT did show better results in both enzymatic convertibility and fermentation, but evaluated on the overall ethanol yield the low-tech pretreatment methods are viable alternatives with similar levels to the HTT (13.4–15.2 g ethanol per 100 g TS raw material).
Comparison of Different Strategies for Selection/Adaptation of Mixed Microbial Cultures Able to Ferment Crude Glycerol Derived from Second-Generation Biodiesel

Objective of this study was the selection and adaptation of mixed microbial cultures (MMCs), able to ferment crude glycerol generated from animal fat-based biodiesel and produce building-blocks and green chemicals. Various adaptation strategies have been investigated for the enrichment of suitable and stable MMC, trying to overcome inhibition problems and enhance substrate degradation efficiency, as well as generation of soluble fermentation products. Repeated transfers in small batches and fed-batch conditions have been applied, comparing the use of different inoculum, growth media, and Kinetic Control. The adaptation of activated sludge inoculum was performed successfully and continued unhindered for several months. The best results showed a substrate degradation efficiency of almost 100% (about 10 g/L glycerol in 21 h) and different dominant metabolic products were obtained, depending on the selection strategy (mainly 1,3-propanediol, ethanol, or butyrate). On the other hand, anaerobic sludge exhibited inactivation after a few transfers. To circumvent this problem, fed-batch mode was used as an alternative adaptation strategy, which led to effective substrate degradation and high 1,3-propanediol and butyrate production. Changes in microbial composition were monitored by means of Next Generation Sequencing, revealing a dominance of glycerol consuming species, such as Clostridium, Klebsiella, and Escherichia.

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Complex interplay of future climate levels of CO₂, ozone and temperature on susceptibility to fungal diseases in barley

Barley (Hordeum vulgare) was grown in different climatic environments with elevated [CO₂] (700 vs 385 ppm), [O₃] (60/90 vs 20 ppb) and temperature (24/19 vs 19/12°C day/night) as single factors and in combinations, to evaluate the impact of these climatic factors on photosynthesis and susceptibility to powdery mildew and spot blotch disease. No significant increase in net CO₂ assimilation rate was observed in barley grown under elevated [CO₂] at ambient temperature. However, this rate was positively stimulated under elevated temperature together with a slightly higher potential quantum efficiency of PSII, both at ambient and elevated [CO₂], suggesting that photosynthesis was not limited by [CO₂] at ambient temperature. When growing under elevated temperature or [O₃], infection by the biotrophic powdery mildew fungus decreased, whereas disease symptoms and growth of the toxin-secreting hemibiotrophic spot blotch fungus increased compared to ambient conditions, implying that climate-induced changes in disease severity could be linked to the trophic lifestyle of the pathogens. Elevated [CO₂] decreased powdery mildew infection but had no effect on spot blotch disease compared to ambient condition. However, the effect of elevated [CO₂], [O₃] and temperature did not act in an additive manner when combined. This led to a surprising disease development in the combination treatments, where powdery mildew infection increased despite the individual reducing effect of the climatic factors, and spot blotch disease decreased despite the individual promoting effect of temperature and ozone, emphasizing the importance of conducting multifactorial experiments when evaluating the potential effects of climate change.
Climate change, CO₂, Ozone, Photosynthesis, Powdery Mildew, Spot blotch

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Refrigerants are widely used in household and industrial applications, such as processes for energy transfer from low grade heat sources. Refrigerants are utilized in heat pump cycles for moving heat from one source to another with the task
to heat or to refrigerate. Environmental issues have been a driving force for the industry to continuously seek novel refrigerants as current refrigerants risk phasing out due to environmental regulations. This trend has been seen since the Kyoto Protocol in 1997 and recently from the EU regulations from 2014, which will restrict the use of some known refrigerants today (Mota-Babiloni et al., 2015). However, design of new refrigerants poses a great challenge and finding an optimum solution for a given application often faces trade-off issues between cycle performance and environmental criteria. In addition, following issues are still to be addressed. What target properties and needs should carefully be selected for a given heat pump cycle to ensure that an optimum refrigerant is found? How can cycle performance and environmental criteria be integrated at the product design stage and not in post-design analysis? Computer-aided product design methods enable the possibility of designing novel molecules, mixtures and blends, such as refrigerants through a systematic framework (Cignitti et al., 2015; Yunus et al., 2014). In this presentation a computer-aided framework is presented for chemical product design through mathematical optimization. Here, molecules, mixtures and blends, are systematically designed through a decomposition based solution method. Given a problem definition, computer-aided molecular design (CAMD) problem is defined, which is formulated into a mixed integer nonlinear program (MINLP). The decomposed solution method then sequentially divides the MINLP into smaller sub-problems; (i) MILP for molecular structure generation, (ii) LP for pure property constraints, (iii) NLP for mixture/blend constraints, (iv) NLP for process constraints. With this, it is ensured that the MINLP is feasible to solve and that a global optimum is reachable. The method is applied on refrigerant design for a heat pump cycle. It is shown how the presented framework can generate optimal novel refrigerants that are high performing and environmentally friendly. This is achieved through integrated product-process based optimization objective, namely, target physicochemical and environmental properties for refrigerant design and target heat pump cycle performance.

Computer-aided Framework for Design of Pure, Mixed and Blended Products

Design of novel chemical products with process and application considerations is an emerging topic in the field of chemical and biochemical engineering. Methods, such as Computer Aided Molecular Design (CAMD) [1] and Computer-aided Mixture and Blend Design (CAMbD) [2], provide the possibility of designing such products. However, these product design problems can quickly become large and difficult, if not infeasible, to solve through mathematical optimization. In addition, considerations of process, application, special product attributes, economic feasibility, environmental and sustainability metrics that must be included in today’s product designs, consequently makes the problem harder to mathematically formulate and to solve. In this work, a framework for computer-aided design of pure, mixed and blended chemical products has been developed. The framework is a systematic approach to formulate and solve CAMbD problems through four sequential steps. In the first step, the needs, target properties and product type are defined. In the second step, the CAMbD is formulated together with objectives and process/application model. In the third step, the formulation is then converted into a mixed integer non-linear program (MINLP). In step four, the MINLP is directly solved (if possible) or sequentially solved through a decomposed optimization approach. The decomposed approach can solve a large MINLP by decomposing it into a smaller set of sub-problems. The framework application is highlighted through a solvent design case study.
Computer-aided Framework for Design of Pure, Mixed and Blended Products

This paper presents a framework for computer-aided design of pure, mixed and blended chemical based products. The framework is a systematic approach to convert a Computer-aided Molecular, Mixture and Blend Design (CAMbD) formulation, based on needs and target properties, into a mixed integer non-linear program (MINLP). The MINLP is sequentially solved through a decomposed optimization approach to solve the possibly large MINLP in a smaller set of sub-problems. The framework application is highlighted through a solvent design case study.

Computer-aided Framework for Synthesis, Design and Retrofit of Wastewater Treatment Plants

Water is used for several purposes in houses and industrial applications, which results in the generation of considerable amounts of wastewater. Wastewater should be handled appropriately which is required from legal, environmental as well as economic and societal perspectives. Wastewater treatment plant (WWTP) design is a formidable challenge. One of the key steps involved is the process synthesis - defined as the selection of treatment processes as a combination of unit operations and processes to create the process flow diagram. As a consequence of the emerging technological developments and resulting increase in the number of alternative wastewater treatment technologies, as well as stricter effluent limit values imposed by regulations; it became increasingly harder to identify the most feasible decision regarding the WWTP network design. Retrofitting of existing treatment plants can also be formulated as a process synthesis challenge in the sense that a new task can be added to the existing treatment line or one or several existing processes can be changed as a result of the emerging needs. Existing plants need retrofitting due to a number of reasons such as: change in the wastewater flow and composition, change in the effluent limitations, as well as changes in the wastewater treatment trends, e.g. from nutrient removal to nutrient recovery. Similarly, recovery possibilities for clean water, energy and materials shifted the perception about wastewater towards being a valuable resource rather than being a waste. While the regulations change to impose stricter effluent limit values for the contaminants, the increasing population and the size of the cities put a barrier on the expansion of the existing WWTPs. Therefore, the retrofitting task has become a complex integrated decision making problem where a number of aspects have to be accounted for in the early stage decision making. The framework has been implemented as a tool which consists of the superstructure covering all relevant treatment alternatives and a database storing design parameters and performances for each alternative technology. The solution of the optimization problem provides an optimal process selection and the optimal flows through the selected network. Finally, the framework is applied to two case studies constituting typical examples for the different scales of wastewater treatment design (BSM2) and
retrofitting studies (Lynetten WWTP of 750,000 PE, and Avedøre WWTP of 265,000 PE) in order to highlight and validate the use of the developed methodology and database.

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**Computer-aided modelling template: Concept and application**
Modelling is an important enabling technology in modern chemical engineering applications. A template-based approach is presented in this work to facilitate the construction and documentation of the models and enable their maintenance for reuse in a wider application range. Based on a model decomposition technique which identifies generic steps and workflow involved, the computer-aided template concept has been developed. This concept is implemented as a software tool, which provides a user-friendly interface for following the workflow steps and guidance through the steps providing additional information and comments on model construction, storage and future use/reuse. The application of the tool is highlighted with a multi-scale modelling case study involving a catalytic membrane fixed bed reactor and a two-phase system for oxidation of unsaturated acid with hydrogen peroxide. Both case studies reflect different aspects of template creation and use with respect to model development.

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Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Publication date: 2015
Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Computer-Aided Process Analysis for the Biocatalytic Production of an Antimicrobial Active Chemical

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, BRAIN AG
Authors: Seita, C. S. (Intern), Rehdorf, J. (Ekstern), Woodley, J. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Computer-aided tool for solvent selection in pharmaceutical processes: Solvent swap

In the pharmaceutical processes, solvents have a multipurpose role since different solvents can be used in different stages (such as chemical reactions, separations and purification) in the multistage active pharmaceutical ingredients (APIs) production process. The solvent swap and selection tasks are important factors in API production. The solvent swap problem is defined as the process where a swap solvent is added to the original solvent solution and the original solvent finally is removed by distillation or liquid-liquid extraction. The selection of an appropriate solvent for each process step is usually based on experience where knowledge-based methods could be employed. However, because of economical, safety and environmental concerns, the use of solvent selection guides together with model-based verification is a better option. Gani et al. (2006) have proposed a computer-aided framework where the solvent selection problem can be solved considering all the concerns mentioned above. The solvent swap problem can be treated as a special solvent selection (Gani et al., 2006) problem together with additional criteria consideration, involving VLE (vapour-liquid equilibria) and LLE (liquid-liquid equilibria). The application of the developed model-based framework is highlighted through several cases studies published in the literature. In the current state, the framework is suitable for problems where the original solvent is exchanged by distillation. A solvent selection guide for fast of suitable swap solvents is developed and is used to retrieve information for the most commonly used solvent candidates typically found in the pharmaceutical industry. The selection is verified by simulation. The framework for the solvent selection and solvent swap is part of an integrated computer-aided framework with the objective to assist the pharmaceutical industry in gaining better process understanding. A software interface to improve the usability of the tool has been created also.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Papadakis, E. (Intern), K. Tula, A. (Intern), Gernaey, K. V. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from 10th European Congress of Chemical Engineering, Nice, France.
Main Research Area: Technical/natural sciences
Green solvent, Process modelling, Process system engineering, Separation
Source: PublicationPreSubmission
Source-ID: 118984790
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Conceptual framework for model-based analysis of residence time distribution in twin-screw granulation

Twin-screw granulation is a promising continuous alternative for traditional batchwise wet granulation processes. The twin-screw granulator (TSG) screws consist of transport and kneading element modules. Therefore, the granulation to a large extent is governed by the residence time distribution within each module where different granulation rate processes dominate over others. Currently, experimental data is used to determine the residence time distributions. In this study, a conceptual model based on classical chemical engineering methods is proposed to better understand and simulate the residence time distribution in a TSG. The experimental data were compared with the proposed most suitable conceptual model to estimate the parameters of the model and to analyse and predict the effects of changes in number of kneading discs and their stagger angle, screw speed and powder feed rate on residence time. The study established that the kneading block in the screw configuration acts as a plug-flow zone inside the granulator. Furthermore, it was found that a balance between the throughput force and conveying rate is required to obtain a good axial mixing inside the twin-screw granulator. Although the granulation behaviour is different for other excipients, the experimental data collection and modelling methods applied in this study are generic and can be adapted to other excipients.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, VTT Tech Res Ctr, Opt Measurement Technol, Kuopio, Finland, Ghent University, VTT - Technical Research Centre of Finland
Pages: 25-34
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: European Journal of Pharmaceutical Sciences
Volume: 71
ISSN (Print): 0928-0987
Ratings:
Continuous Catalytic Hydrodeoxygenation of Guaiacol over Pt/SiO₂ and Pt/H-MFI-90

Hydrodeoxygenation of guaiacol in the presence of 1-octanol was studied in a fixed-bed reactor under mild conditions (50–250 °C) over platinum particles supported on silica (Pt/SiO₂) and a zeolite with framework type MFI at a Si/Al-ratio of 45 (Pt/H-MFI-90). The deoxygenation selectivity strongly depended on the support and the temperature. Both guaiacol and octanol were rapidly deoxygenated in the presence of hydrogen over Pt/H-MFI-90 at 250 °C to cyclohexane and octane, respectively. In contrast, Pt/SiO₂ mostly showed hydrogenation, but hardly any deoxygenation activity. The acidic sites of the MFI-90 support lead to improved deoxygenation performance at the mild temperature conditions of this study.
Significant conversions under reaction conditions applied already occurred at temperatures of 200 °C. However, during long-term stability tests, the Pt/H-MFI-90 catalyst deactivated after more than 30 h, probably due to carbon deposition, whereas Pt/SiO₂ was more stable. The catalytic activity of the zeolite catalyst could only partly be regained by calcination in air, as some of the acidic sites were lost.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Karlsruhe Institute of Technology KIT
Authors: Hellinger, M. (Ekstern), Baier, S. (Ekstern), Mortensen, P. M. (Intern), Kleist, W. (Ekstern), Jensen, A. D. (Intern), Grunwaldt, J. (Ekstern)
Pages: 1152-1166
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Catalysts
Volume: 5
Issue number: 3
ISSN (Print): 2073-4344
Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.44 SJR 0.928 SNIP 1.217
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.076 SNIP 1.246 CiteScore 3.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.683 SNIP 1.074 CiteScore 2.17
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.521 SNIP 0.582
Scopus rating (2012): SJR 0.471 SNIP 0.358
Original language: English
Electronic versions:
catalysts_05_01152.pdf
DOI:
10.3390/catal5031152
Source: FindIt
Source-ID: 2279639474
Publication: Research - peer-review › Journal article – Annual report year: 2015

**Controlled release in hard to access places by poly(methyl methacrylate) microcapsules triggered by gamma irradiation**
Gamma irradiation was investigated as a triggering stimulus for the activation of poly(methyl methacrylate) (PMMA) microcapsules. PMMA was exposed to varying doses of irradiation and analyzed by differential scanning calorimetry, size-exclusion chromatography, and nuclear magnetic resonance. It was found that the glass transition temperature (Tg) of the polymer decreases at low irradiation doses. Additionally, Tg can be physically adjusted by adding a plasticizer, and both kinds of microcapsules were successfully prepared with non-plasticized and plasticized PMMA shell. Finally, impermeable microcapsules were shown to become permeable after irradiation and release an encapsulated cross-linker, which enables the remotely controlled formation of polydimethylsiloxanes in traditionally unavailable places. Therefore, the activation method has significant implications for industrial application.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Maersk Oil Research and Technology Centre
Authors: Kostrzewska, M. (Intern), Ma, B. (Intern), Javakhishvili, I. (Intern), Hansen, J. H. (Ekstern), Hvilsted, S. (Intern), Skov, A. L. (Intern)
Pages: 1059-1064
Control of a post-combustion CO₂ capture plant during process start-up and load variations

Dynamic and flexible operation of a carbon capture plant is important as thermal power plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar energy. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Moreover, we implement a decentralized proportional-integral (PI) based control scheme and we evaluate the performance of the control structure for various operational procedures, e.g. start-up, load changes, noise on the flue gas flow rate and composition. Note that the carbon capture plant is based on the solvent storage configuration. To the authors' knowledge, this is the first paper addressing the issue of start-up operation and control of carbon capture. The study demonstrates that the implemented control structure keeps the carbon capture process at 90% CO₂ removal rate with a deviation up to 8% during load variations. In addition, it reveals that the control structure brings the process to the desired set point in approximately 10 min during process start-up. [All rights reserved Elsevier].

General information
State: Published
Organizations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Gaspar, J. (Intern), Jørgensen, J. B. (Intern), Fosbøl, P. L. (Intern)
Pages: 580-585
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Main Research Area: Technical/natural sciences
Conference: 9th International Symposium on Advanced Control of Chemical Processes, Whistler, Canada, 07/06/2015 - 07/06/2015
Process applications, Energy processes and control, Modeling and identification
Electronic versions:
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Source: FindIt
Source-ID: 277547506
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

Control of a post-combustion CO₂ capture plant during process start-up and load variations

Dynamic and flexible operation of a carbon capture plant is important as thermal power plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar energy. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Moreover, we implement a decentralized proportional-integral (PI) based control scheme and we evaluate the performance of the control structure for various operational procedures, e.g. start-up, load changes, noise on the flue gas flow rate and composition. Note that the carbon capture plant is based on the solvent storage configuration. To the authors' knowledge, this is the first paper addressing the issue of start-up operation and control of carbon capture. The study demonstrates that the implemented control structure keeps the carbon capture process at 90% CO₂ removal rate with a deviation up to 8% during load variations. In addition, it reveals that the control structure brings the process to the desired set point in approximately 10 min during process start-up.
Control of Bioprocesses

The purpose of bioprocess control is to ensure that the plant operates as designed. This chapter presents the fundamental principles for control of biochemical processes. Through examples, the selection of manipulated and controlled variables in the classical reactor configurations is discussed, so are control objectives and the challenges in obtaining good control of the bioreactor. The objective of this chapter is to discuss the bioreactor control problems and to highlight some general traits that distinguish operation of bioprocesses from operation of processes in the conventional chemical process industries. It also provides a number of typical control loops for different objectives. A brief introduction to the general principles of process control, the PID control algorithm is discussed, and the design and effect of tuning are shown in an example. Finally, a discussion of novel, model-free control approaches for bioreactors is provided.

Control Structure Design for an EBP2R Process Operated as a Sequencing Batch Reactor

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Valverde Perez, B. (Intern), Fuentes-Martínez, J. M. (Ekstern), Flores Alsina, X. (Intern), Wágner, D. S. (Intern), Huusom, J. K. (Intern), Plósz, B. G. (Intern)
Number of pages: 1
Publication date: 2015
Event: Poster session presented at 9th IWA Symposium on Systems Analysis and Integrated Assessment (Watermatex 2015), Gold Coast, Queensland, Australia.
Control Structure Design of an Innovative Enhanced Biological Nutrient Recovery Activated Sludge System Coupled with a Photobioreactor

The TRENS system is a train of biological units designed for resource recovery from wastewater. It is a sequence of a modified enhanced biological phosphorus removal and recovery system (EBP2R) coupled with a photobioreactor (PBR). The bacteria-based system constructs an optimal culture media for the downstream algae cultivation. In this work, we present a control strategy to ensure an optimal nutrient balance to feed to the PBR, so the grown algal suspension is suitable for fertigation (irrigation and fertilization of agricultural crops). The system is able to recover up to 75% of the influent load, while keeping an optimal N-to-P ratio of 16 in the influent to the PBR. The system is tested under different scenarios, where the influent quality is disturbed following a step change. The control system is able to reject most of the disturbances. However, when the P-recovery is limited by the bacteria in the reactor, the control system is not able to keep the optimal phosphorus load, but only the optimal percentage recovery from the influent phosphorus. In this scenario, the system is kept under optimal conditions – in terms of nutrient balance – because the N-to-P ratio is still at 16, so the green microalgae can take up most of the incoming nutrients into the PBR. The control system is able to keep the optimal phosphorus load during dynamic conditions. However when the influent nitrogen is limiting the process, the N-to-P ratio drops under the optimal value. Further research is needed in order to assess the controllability of the PBR and the possible impact on the upstream operation conditions.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
Authors: Valverde Perez, B. (Intern), Fuentes-Martínez, J. M. (Ekstern), Flores Alsina, X. (Intern), Gernaey, K. (Intern), Huusom, J. K. (Intern), Plósz, B. G. (Intern)
Pages: 2555–2560
Publication date: 2015
Conference: 25th European Symposium on Computer Aided Process Engineering, Copenhagen, Denmark, 31/05/2015 - 31/05/2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Computer - Aided Chemical Engineering
Volume: 37
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.48 SJR 0.198 SNIP 0.215
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.245 SNIP 0.249 CiteScore 0.39
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.239 SNIP 0.217 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.216 SNIP 0.175 CiteScore 0.28
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.196 SNIP 0.267 CiteScore 0.33
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.194 SNIP 0.199 CiteScore 0.3
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.181 SNIP 0.135
Scopus rating (2009): SJR 0.16 SNIP 0.163
Scopus rating (2008): SJR 0.167 SNIP 0.124
Cubic Plus Association Equation of State for Flow Assurance Projects

Thermodynamic hydrate inhibitors such as methanol, ethanol, (mono) ethylene glycol (MEG), and triethylene glycol (TEG) are widely used in the oil and gas industry. On modeling these compounds, we show here how the CPA equation of state was implemented in an in-house process simulator as an in-built model. To validate the implementation, we show calculations for binary systems containing hydrate inhibitors and water or hydrocarbons using the Cubic Plus Association (CPA) and Soave-Redlich-Kwong (SRK) equation of states, also comparing against experimental data. For streams containing natural gas and water, CPA was applied to calculate the loss of the inhibitor to the vapor phase as a function of temperature and pressure. Simulations of dehydration units using TEG were conducted, and the CPA results were compared with that of two commercial simulators which used their available thermodynamic packages for glycol applications, proving that the CPA calculations are in good agreement with these models and showing that this is an adequate way to simulate complex matures containing natural gas, water, and hydrate inhibitors.

General information

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Universidade Federal do Rio de Janeiro, Petrobras, Universidade Federal Fluminense
Authors: dos Santos, L. C. (Ekstern), Abunahman, S. S. (Ekstern), Tavares, F. W. (Ekstern), Ruiz Ahon, V. R. (Ekstern), Kontogeorgis, G. M. (Intern)
Pages: 6812-6824
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Industrial and Engineering Chemistry Research
Volume: 54
Issue number: 26
ISSN (Print): 0888-5885
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BFI (2018): BFI-level 2
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Deactivation of SCR catalysts in biomass fired power plants

In order to meet national and European targets regarding reduction of the emission of greenhouse gases, fossil fuels are gradually being substituted with biomass, such as straw, wood chips and wood pellets, in Danish combined heat and power plants. The release of inorganic elements, present in such biomass fuels, however, causes enhanced strain on the different equipment in these power plants. One of the affected units is the catalyst for selective catalytic reduction (SCR) of nitrogen oxides, which undergoes accelerated deactivation due to deposition of potassium rich particles and subsequent poisoning. The potassium poisoning of commercial vanadia based SCR catalysts have been studied for more than two decades, and a broad understanding have been obtained. However, more detailed information on the overall mechanism of deposition, reaction and transport of potassium, and its function of catalyst composition and operating conditions, is not available. The main objective of the work presented in this thesis has been to conduct an in depth investigation of the deactivation mechanism of vanadia based SCR catalysts, when subjected to potassium rich aerosols. It has furthermore
been a goal to suggest and test new alkali resistant catalyst formulations, coatings and/or improved means of operation which can extend the life-time of SCR catalysts in biomass fired power plants. Plate-type V₂O₅-(WO₃)/TiO₂ SCR catalysts have been exposed to KCl and K₂SO₄ aerosols in a bench-scale reactor at 150, 300 or 350 °C for up to 600 hours. The activity of fresh and exposed catalysts was measured in the temperature range 250-400 °C in a laboratory-scale reactor. All samples exposed for more than 240 hours proved to have deactivated significantly, however, catalysts exposed at 150 °C showed higher remaining activity compared to samples exposed at 300-350 °C. This indicates that the deactivation rate increases with the exposure/operating temperature. The majority of the catalysts exposed to KCl aerosols at high temperatures had lost more than 90 % of their initial activity. Increasing the mode of the mass based KCl particle size distribution, from an aerodynamic diameter of 0.12 to 2.6 μm, showed no effect on the catalyst deactivation rate. This may be attributed to a continued presence of a significant number of ultrafine KCl particles in the flue gas. The K₂SO₄ aerosols caused a slower rate of deactivation compared to the KCl aerosols. This indicates that potassium bound in K₂SO₄ deposits, on the catalyst surface, is less mobile than that bound KCl. However, an effect of particle size on the catalyst deactivation cannot be excluded, as the obtained K₂SO₄ aerosols generally were shifted towards larger particles (mass based distribution mode: 1.3 μm) compared to the KCl aerosols. Activity measurements on the exposed catalysts indicated that WO3 promoted samples, which in general showed higher NH₃ adsorption capacities, had lost larger fractions of their initial activities compared to unpromoted ones. This is likely due to the enhanced Brønsted acidity which appears to facilitate the transport of potassium in SCR catalysts. The potassium mobility has further been studied using a new experimental protocol. This involves two-layer pellets of vanadia based SCR catalysts, where one side has been impregnated with KCl or K₂SO₄. SEM-WDS measurements on pellets heat treated at 350 °C showed that potassium bound in KCl readily left its counter ion, causing a faster transport into the undoped catalyst compared to potassium from K₂SO₄. Furthermore, only half of the sulfate bound potassium seemed to be able to leave its solid matrix. These observations are in agreement with the results from the plate exposure experiments. Likewise as indicated by the bench-scale experiments, the presence of WO₃ in the two-layer pellets appeared to facilitate the potassium transport. The potassium blocking abilities of potential coating materials have been tested using three-layer pellets. Here, layers of MgO, sepiolite, a mixture of the two, or Hollandite manganese oxide have been introduced in between the two (respectively potassium impregnated and undoped) catalyst layers. Pure MgO proved to be the most effective barrier of the tested candidates, and was able to retain the potassium in the impregnated side of the pellet, even after 7 days of exposure at SCR conditions. Partial or full potassium penetration of layers of the other tested materials was observed. Half-length monoliths have been exposed to KCl aerosols in the bench-scale setup at 350 °C for up to 1100 hours, and their activities were followed by in situ measurements. A 3%V₂O₅-7%WO₃/TiO₂ reference catalyst deactivated with a rate of 0.91 %/day during 960 hours of exposure, and a subsequent SEM-EDS analysis showed complete potassium penetration of the catalyst wall with average K/V molar ratios of 0.38-0.51. During 1100 hours of exposure, a similar monolith coated with 8.06 wt.% MgO deactivated with a rate of 0.24 %/day, relative to the fresh activity of the reference, but showed a 42 % lower start activity due to enhanced transport limitations. The MgO coat proved to have protected the SCR catalyst against potassium poisoning, however, SEM-EDS analysis showed that some potassium had penetrated the coat. The SEM analysis also indicated that the MgO coat was rather fragile and adhered weakly to the catalyst substrate, indicating the need for a binder material. A catalyst coated with a 1:1 mixture of MgO and TiO₂ showed insufficient start activity (30 % of that of the reference) when tested in the bench-scale setup, likely due to a low porosity of the coat. V₂O₅ deactivation model describing the potassium poisoning of an SCR monolith catalyst has been derived. The model accounts for deposition and consumption of potassium rich particles on the external catalyst surface, the build-up of potassium, bound to Brønsted acid sites, throughout the catalyst wall, and the resulting loss in SCR activity. Simulations show that the particle deposition rate, and hence the deactivation rate, decreases if the particle size of the incoming aerosol is increased. The results obtained in this work indicate that the life-time of SCR catalysts used in biomass fired power plants can be improved by ensuring a high conversion of KCl to K₂SO₄ aerosols, by reducing the operating temperature, and by increasing the size of the incoming, potassium rich aerosol particles to above 200 nm. While it may not be mechanically durable in its current state of development, applying an MgO coat to the SCR catalyst will also protect it against potassium poisoning.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Olsen, B. K. (Intern), Castellino, F. (Intern), Jensen, A. D. (Intern)
Number of pages: 140
Publication date: 2015

Publication information
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PhD_thesis_Brian_Kj_rgaard_Olsen.pdf
Source: PublicationPreSubmission
Source-ID: 116994975
Publication: Research › Ph.D. thesis – Annual report year: 2015
De danske kraftværkers omstilling fra kul til biomasse
Det er målet at sikre en energi- og kosteffektiv omstilling frem mod fuldstændig udfasning af kul på de danske kraftvarmeværker i 2030. For at støtte denne omstilling er der gennemført et ph.d.-projekt, som har fokuseret på modellering af biostøvflammer.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Johansen, J. M. (Intern), Jensen, P. A. (Intern), Glarborg, P. (Intern)
Pages: 22-25
Publication date: 2015
Main Research Area: Technical/natural sciences

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Journal: Dansk Kemi
Volume: 96
Issue number: 10
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: English
Electronic versions:
DAK10_2015s22_251.pdf
Publication: Research › Journal article – Annual report year: 2015

Projects:

Tubular membrane reactions for immobilization of enzymes
Department of Chemical and Biochemical Engineering
Period: 01/03/2018 → 28/02/2021
Number of participants: 4
Phd Student:
Zverina, Libor (Intern)
Supervisor:
Pinelo, Manuel (Intern)
Woodley, John (Intern)
Main Supervisor:
Daugaard, Anders Egede (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Caoting with inherent sensing functionality based on dielectric elastomers
Department of Chemical and Biochemical Engineering
Period: 01/02/2018 → 31/01/2021
Number of participants: 3
Phd Student:
Krpovic, Sara (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Heavy Duty Coatings

Department of Chemical and Biochemical Engineering
Period: 01/02/2018 → 31/01/2021
Number of participants: 4
Phd Student:
Ekbrant, Björn Erik Fristrup (Intern)
Supervisor:
Ambat, Rajan (Intern)
Paulsen, Andreas Lundtang (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD

Optimization of industriel anaerobic pre-treatment processes

Department of Chemical and Biochemical Engineering
Period: 01/02/2018 → 31/01/2021
Number of participants: 5
Phd Student:
Monje López, Vicente Tomás (Intern)
Supervisor:
Flores Alsina, Xavier (Intern)
Junicke, Helena (Intern)
Krühne, Ulrich (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Production of Polyhydroxyalkanoates from crude glycerol

Department of Chemical and Biochemical Engineering
Period: 01/02/2018 → 31/01/2020
Number of participants: 4
Phd Student:
Burniol Figols, Anna (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Skiadas, Ioannis V (Intern)
Main Supervisor:
Gavala, Hariklia N. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD
Structure property relationships in coatings
Department of Chemical and Biochemical Engineering
Period: 01/02/2018 → 31/01/2021
Number of participants: 4
Phd Student:
Juraskova, Alena (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Olsen, Stefan Møller (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Ecological Control Strategies for Biobutanol Production
Department of Chemical and Biochemical Engineering
Period: 01/01/2018 → 31/12/2020
Number of participants: 5
Phd Student:
Pinto, Tiago Nuno Baptista Castro (Intern)
Supervisor:
Alsina, Xavier Flores (Ekstern)
Junicke, Helena (Intern)
Eliasson Lantz, Anna (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Gas liberation in tight porous medium
Department of Chemical and Biochemical Engineering
Period: 01/01/2018 → 31/12/2020
Number of participants: 4
Phd Student:
Al-Masri, Wael Fadi (Intern)
Supervisor:
Nielsen, Carsten Møller (Intern)
Nielsen, Sidsel Marie (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Strechable conductive elastosmers
Department of Chemical and Biochemical Engineering
Period: 01/01/2018 → 31/12/2020
Number of participants: 3
Phd Student:
Shao, Jiang (Intern)
Theory, simulation and models for electrolyte systems with focus on ionic liquids

Department of Chemical and Biochemical Engineering
Period: 01/01/2018 → 31/12/2020
Number of participants: 4
Phd Student:
Tong, Jiahuan (Intern)
Supervisor:
Liang, Xiaodong (Intern)
Zhang, Suo-Jiang (Ekstern)
Main Supervisor:
von Solms, Nicolas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Methane production and carbon capture through hydrate swapping

Department of Chemical and Biochemical Engineering
Period: 01/12/2017 → 30/11/2020
Number of participants: 3
Phd Student:
Shi, Meng (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
von Solms, Nicolas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Study on self-hearing and high-permittivity silicone elastomer/keratin composite materials

Department of Chemical and Biochemical Engineering
Period: 01/12/2017 → 30/11/2020
Number of participants: 4
Phd Student:
Liu, Xue (Intern)
Supervisor:
Nie, Yi (Ekstern)
Zhang, Suo-Jiang (Ekstern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD
Catalytic Cracking of Sugars for Production of Chemicals

Department of Chemical and Biochemical Engineering
Period: 01/11/2017 → 31/10/2020
Number of participants: 4
Phd Student:
Schandel, Christian Bækhøj (Intern)
Supervisor:
Høj, Martin (Intern)
Osmundsen, Christian Mårup (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Catalytic methanol synthesis

Department of Chemical and Biochemical Engineering
Period: 01/11/2017 → 31/10/2020
Number of participants: 3
Phd Student:
Nielsen, Niels Dyreborg (Intern)
Supervisor:
Jensen, Anker Degn (Intern)
Main Supervisor:
Christensen, Jakob Munkholt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

Continuous Biocatalytic Alkene Hydrogenation

Department of Chemical and Biochemical Engineering
Period: 01/11/2017 → 31/10/2020
Number of participants: 4
Phd Student:
Lindeque, Rowan Malan (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Krühne, Ulrich (Intern)
Main Supervisor:
Woodley, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Novel catalysts for the oxidation of methanol to formaldehyde

Department of Chemical and Biochemical Engineering
Period: 01/11/2017 → 31/10/2020
Number of participants: 4
Phd Student:
Thrane, Joachim (Intern)
Supervisor:
Høj, Martin (Intern)
Thorhauge, Max (Ekstern)

Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Solvent Molecular Design Process Synthesis and Energy Requirements in Chemical and Biochemical Processes
Department of Chemical and Biochemical Engineering
Period: 01/11/2017 → 31/10/2020
Number of participants: 4
Phd Student:
Chen, Yuqiu (Ekstern)
Supervisor:
Gani, Rafiqul (Intern)
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Woodley, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Air-pollutant sensor system for wood slopes
Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Du, Yifan (Ekstern)
Supervisor:
Clausen, Sønnik (Intern)
Illerup, Jytte Boll (Intern)
Main Supervisor:
Glarborg, Peter (Intern)

Financing sources
Air-pollutant sensor system for wood stoves

Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Du, Yifan (Intern)
Supervisor:
Clausen, Sønnik (Intern)
Illerup, Jytte Boll (Intern)
Main Supervisor:
Glarborg, Peter (Intern)

Financing sources

Anticorrosive coatings and pigments engineering

Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Sedaghat Nezhad, Sina (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources

Coating interlayer adhesion loss

Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Wang, Ting (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources

Development and Application of Novel Free-floating Sensor Device for Bioprocess Optimization

Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 5
Phd Student:
Bisgaard, Jonas (Intern)
Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Skyggebjerg, Ole (Intern)
Skyggebjerg, Ole (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD

Functional Polysilazanes for Coating Applications

Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/01/2018
Number of participants: 4
Phd Student:
Kristiansen, Thomas (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Daugaard, Anders Egede (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Kinetics of Scale Formation in Oil and Gas Production

Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Lomsøy, Petter (Intern)
Supervisor:
Ambat, Rajan (Intern)
Fosbøl, Philip Loldrup (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Membrane-based in-situ product removal

Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Jaksland, Anders (Intern)
Supervisor:
Pinelo, Manuel (Intern)
Wan, Yinhua (Ekstern)
Main Supervisor:
Woodley, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

NOx control in combustion of alternative fuels
Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Krum, Kristian Røhe Kongsted (Intern)
Supervisor:
Norman, Thomas (Intern)
Wu, Hao (Intern)
Main Supervisor:
Glarborg, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Coatings for high pressure and high temperature
Department of Chemical and Biochemical Engineering
Period: 15/08/2017 → 14/08/2020
Number of participants: 4
Phd Student:
Ferrero, Gianni (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Advanced wound care adhesives with new functional properties
Department of Chemical and Biochemical Engineering
Period: 01/08/2017 → 31/07/2020
Number of participants: 6
Phd Student:
Chiaula, Valeria (Intern)
Supervisor:
Mazurek, Piotr Stanislaw (Intern)
Nielsen, Anders Christian (Ekstern)
Torneø, Jens (Intern)
Torneø, Jens (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)

Financing sources
Synthesis and characterization of hydrogels to be used as dielectric elastomers

Department of Chemical and Biochemical Engineering
Period: 15/07/2017 → 14/07/2020
Number of participants: 3
PhD Student:
Vaicekauskaite, Justina (Intern)
Supervisor:
Yu, Liyun (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

High performance immobilization of enzymes in inorganic membranes

Department of Chemical and Biochemical Engineering
Period: 01/06/2017 → 31/05/2020
Number of participants: 4
PhD Student:
Sigurdardóttir, Sigyn Björk (Intern)
Supervisor:
Della Negra, Michela (Intern)
Kaiser, Andreas (Intern)
Main Supervisor:
Pinelo, Manuel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Sustainable Process Synthesis and Design

Department of Chemical and Biochemical Engineering
Period: 01/05/2017 → 30/04/2020
Number of participants: 4
PhD Student:
Al, Resul (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Zubov, Alexandr (Intern)
Main Supervisor:
Sin, Gürkan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Discovery and engineering of new enzymes for efficient enzymatic conversion of CO2 to CH2OH

Department of Chemical and Biochemical Engineering
Period: 01/04/2017 → 31/03/2020
Number of participants: 4
Phd Student:
Nielsen, Christian Førgaard (Intern)
Supervisor:
Christensen, Jakob Munkholt (Intern)
Lange, Lene (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Physiological characterization of the impact of gradients on fermentation processes
Department of Chemical and Biochemical Engineering
Period: 01/03/2017 → 29/02/2020
Number of participants: 4
Phd Student:
Nadal Rey, Gisela (Intern)
Supervisor:
Cornelissen, Sjef (Ekstern)
Eliasson Lantz, Anna (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Advanced oil recovery processes: Modifications of injection water composition
Department of Chemical and Biochemical Engineering
Period: 15/02/2017 → 14/02/2020
Number of participants: 3
Phd Student:
Hao, Jiasheng (Intern)
Supervisor:
Shapiro, Alexander (Intern)
Main Supervisor:
Nielsen, Sidsel Marie (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Decolorization, Desalination and Purification of Molasses by Nanofiltration
Department of Chemical and Biochemical Engineering
Period: 15/02/2017 → 15/09/2017
Number of participants: 4
Phd Student:
Tan, Sheng (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Luo, Jianquan (Intern)
Main Supervisor:
Pinelo, Manuel (Intern)

**Financing sources**
- Source: Internal funding (public)
- Name of research programme: Stipendie fra udlandet
- Project: PhD

The Thermodynamics and Transport Properties on Ionic-Liquids Based Compounds

Department of Chemical and Biochemical Engineering
- Period: 15/02/2017 → 14/02/2020
- Number of participants: 3
- Phd Student:
  - Cai, Yingjun (Ekstern)
- Supervisor:
  - von Solms, Nicolas (Intern)
- Main Supervisor:
  - Thomsen, Kaj (Intern)

**Financing sources**
- Source: Internal funding (public)
- Name of research programme: Stipendie fra udlandet
- Project: PhD

CFD Modelling of dynamic microfiltration for application in biotechnology processes

Department of Chemical and Biochemical Engineering
- Period: 01/02/2017 → 31/01/2020
- Number of participants: 4
- Phd Student:
  - Marke, Henrik Sander (Intern)
- Supervisor:
  - Hansen, Ernst (Intern)
  - Pinelo, Manuel (Intern)
- Main Supervisor:
  - Krühne, Ulrich (Intern)

**Financing sources**
- Source: Internal funding (public)
- Name of research programme: Industrial PhD
- Project: PhD

Use of Zeolites for Tar De-Oxygenation

Department of Chemical and Biochemical Engineering
Period: 01/02/2017 → 31/01/2020  
Number of participants: 5  
Phd Student:  
Eschenbacher, Andreas (Intern)  
Supervisor:  
Ahrenfeldt, Jesper (Intern)  
Henriksen, Ulrik Birk (Intern)  
Jensen, Peter Arendt (Intern)  
Main Supervisor:  
Jensen, Anker Degn (Intern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Samfinansieret - Andet  
Project: PhD

Enhanced Oil Recovery Methods targeting Danish North Sea Chalk Reservoirs

Department of Chemical and Biochemical Engineering  
Period: 15/01/2017 → 14/01/2020  
Number of participants: 3  
Phd Student:  
Taheriotaghsara, Mirhossein (Intern)  
Supervisor:  
Shapiro, Alexander (Intern)  
Main Supervisor:  
Nielsen, Sidsel Marie (Intern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU)  
Project: PhD

Advanced Modelling, Simulation and Optimization for in Silico Process Design

Department of Chemical and Biochemical Engineering  
Period: 01/01/2017 → 31/12/2019  
Number of participants: 6  
Phd Student:  
Öner, Merve (Intern)  
Supervisor:  
Abildskov, Jens (Ekstern)  
Gernaey, Krist V. (Intern)  
Shibabaw Molla, Getachew (Intern)  
Stocks, Stuart M. (Ekstern)  
Main Supervisor:  
Sin, Gürkan (Intern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Samfinansieret - Andet  
Project: PhD

Alternative liquid fuels in burners optimized for low NOx emissions and high burn out

Department of Chemical and Biochemical Engineering  
Period: 01/01/2017 → 31/12/2019  
Number of participants: 4  
Phd Student:  
Cafaggi, Giovanni (Intern)  
Supervisor:  

Antimicrobial Polymers for Catheter Coatings
Department of Chemical and Biochemical Engineering
Period: 01/01/2017 → 31/12/2019
Number of participants: 4
PhD Student:
Andersen, Christian (Intern)
Supervisor:
Madsen, Niels Jørgen (Ekstern)
Skov, Anne Ladegaard (Intern)
Main Supervisor:
Daugaard, Anders Egede (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

Conceptual design of yeast propagation strategies for improved bioethanol production
Department of Chemical and Biochemical Engineering
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
PhD Student:
Lopez, Pau Cabañeros (Intern)
Supervisor:
Junicke, Helena (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Mechanical and photochemical stabilization of flexible organic solar cells
Department of Chemical and Biochemical Engineering
Period: 01/01/2017 → 31/12/2019
Number of participants: 4
PhD Student:
Ogliani, Elisa (Intern)
Supervisor:
Hvilsted, Søren (Intern)
Yu, Liyun (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD
Monolithic Thiol-ene Materials with Drastically Different Mechanical Properties

Department of Chemical and Biochemical Engineering
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
Phd Student:
Shen, Peng (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Main Supervisor:
Szabo, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Sustainable Catalytic Alcohol Synthesis from Hydrogen and Carbon Dioxide

Department of Chemical and Biochemical Engineering
Period: 01/01/2017 → 31/12/2019
Number of participants: 4
Phd Student:
Schumann, Max (Intern)
Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Jensen, Anker Degn (Intern)
Main Supervisor:
Christensen, Jakob Munkholt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Homology to peptide pattern for annotation of carbohydrate-active enzymes and prediction of function

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 14/12/2016 → 12/04/2017
Number of participants: 5
Acronym: Hotpep-carbohydrate
Project participant:
Busk, Peter Kamp (Intern)
Pilgaard, Bo (Intern)
Lezyk, Mateusz Jakub (Intern)
Meyer, Anne S. (Intern)
Lange, Lene (Intern)

Advanced modeling, simulation and tools integration for in-silico process design and optimization

Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Period: 01/11/2016 → …
Number of participants: 1
Project participant:
Shibabaw Molla, Getachew (Intern)
**Phase Behavior of Inhomogeneous Fluids**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2016 → 31/10/2019  
Number of participants: 3  
Phd Student: Camacho Vergara, Edgar Luis (Intern)  
Supervisor: Liang, Xiaodong (Intern)  
Main Supervisor: Kontogeorgis, Georgios (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU)  
Project: PhD

**Chemical & Biochemical Sustainable Process Synthesis - Intensification**  
Department of Chemical and Biochemical Engineering  
Period: 15/10/2016 → 14/10/2019  
Number of participants: 4  
Phd Student: Garg, Nipun (Intern)  
Supervisor: Kontogeorgis, Georgios (Intern)  
Main Supervisor: Woodley, John (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansierede - Virksomhed  
Project: PhD

**Development of a Raman spectroscopy based control system for the U-Loop fermentor**  
Department of Chemical and Biochemical Engineering  
Period: 15/10/2016 → 14/10/2019  
Number of participants: 4  
Phd Student: Petersen, Leander Adrian Haaning (Intern)  
Supervisor: Christensen, Ib (Ekstern)  
Eliasson Lantz, Anna (Intern)  
Main Supervisor: Gernaey, Krist V. (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Industrial PhD  
Project: PhD

**Novel testing methods for intumescent coating**  
Department of Chemical and Biochemical Engineering  
Period: 15/10/2016 → 14/10/2019  
Number of participants: 3  
Phd Student:
CFD Simulation of Heterogeneous Reacting Systems

Department of Chemical and Biochemical Engineering
Period: 01/10/2016 → 30/09/2019
Number of participants: 3
PhD Student:
Luo, Hao (Intern)
Supervisor:
Wu, Hao (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Models for estimation and analyses of emissions from chemical processes and products

Department of Chemical and Biochemical Engineering
Period: 01/10/2016 → 30/09/2019
Number of participants: 5
PhD Student:
Jhamb, Spardha Virendra (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Liang, Xiaodong (Intern)
Liang, Xiaodong (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Thermodynamic Modeling of CO2 Gas Hydrate Formation Systems

Department of Chemical and Biochemical Engineering
Period: 01/10/2016 → 30/09/2019
Number of participants: 3
PhD Student:
Sun, Li (Intern)
Supervisor:
Liang, Xiaodong (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
**Development Reactors**

Department of Chemical and Biochemical Engineering  
Period: 15/09/2016 → 14/10/2019  
Number of participants: 4  
PhD Student:  
Svith, Casper Stryhn (Intern)  
Supervisor:  
Lin, Weigang (Intern)  
Wu, Hao (Intern)  
Main Supervisor:  
Dam-Johansen, Kim (Intern)

**Financing sources**

Source: Internal funding (public)  
Name of research programme: Samfinansierede - Virksomhed  
Project: PhD

**Production of alkali from cocoa husk ash and biological extraction of hydrocolloid from Sargassum sp.**

Department of Chemical and Biochemical Engineering  
Center for BioProcess Engineering  
Period: 05/09/2016 → 06/02/2017  
Number of participants: 4  
Project participant:  
Rhein-Knudsen, Nanna (Intern)  
Bentil, Joseph Asankomah (Intern)  
Supervisor:  
Ale, Marcel Tutor (Intern)  
Main Supervisor:  
Meyer, Anne S. (Intern)

**Production of alkali from cocoa husk ash for extraction of hydrocolloid from biologically pretreated red seaweed**

Department of Chemical and Biochemical Engineering  
Center for BioProcess Engineering  
Period: 05/09/2016 → 06/02/2017  
Number of participants: 4  
PhD Student:  
Rhein-Knudsen, Nanna (Intern)  
Bentil, Joseph Asankomah (Intern)  
Supervisor:  
Ale, Marcel Tutor (Intern)  
Main Supervisor:  
Meyer, Anne S. (Intern)

**Relations**

Parent project:  
Seaweed Biorefinery in Ghana  
Project

**Catalytic Oxidation of CH4**

Department of Chemical and Biochemical Engineering  
Period: 01/09/2016 → 31/08/2019  
Number of participants: 4  
PhD Student:
Zhang, Yu (Intern)  
Supervisor:  
Christensen, Jakob Munkholt (Intern)  
Jensen, Anker Degn (Intern)  
Main Supervisor:  
Glarborg, Peter (Intern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Samfinansieret - Andet  
Project: PhD

Downstream Processing of Biochemical Processes  
Department of Chemical and Biochemical Engineering  
Period: 01/09/2016 → 31/08/2019  
Number of participants: 3  
Phd Student:  
Meyer, Kristian (Intern)  
Supervisor:  
Huusom, Jakob Kjøbsted (Intern)  
Main Supervisor:  
Abildskov, Jens (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Samfinansierede - Virksomhed  
Project: PhD

Energy Efficiency Hybrid Separation Process with Ionic Liquid  
Department of Chemical and Biochemical Engineering  
Period: 01/09/2016 → 31/08/2019  
Number of participants: 4  
Phd Student:  
Liu, Xinyan (Intern)  
Supervisor:  
Liang, Xiaodong (Intern)  
Liang, Xiaodong (Intern)  
Main Supervisor:  
Kontogeorgis, Georgios (Intern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Stipendie fra udlandet  
Project: PhD

Fluidized bed combustion of biomass  
Department of Chemical and Biochemical Engineering  
Period: 01/09/2016 → 31/08/2019  
Number of participants: 4  
Phd Student:  
Ulusoy, Burak (Intern)  
Supervisor:  
Lin, Weigang (Intern)  
Wu, Hao (Intern)  
Main Supervisor:  
Dam-Johansen, Kim (Intern)  

Financing sources
A Decision Support Tool for Screening Novel WWT Processes

Department of Chemical and Biochemical Engineering
Period: 15/08/2016 → 14/08/2019
Number of participants: 3
Phd Student:
Behera, Chitta Ranjan (Ekstern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Sin, Gürkan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Optimized recycling in an integrated melting furnace for production of stone wool melt

Department of Chemical and Biochemical Engineering
Period: 01/08/2016 → 17/02/2020
Number of participants: 5
Phd Student:
Schultz-Falk, Vickie (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Hansen, Lars Elmkilde (Ekstern)
Solvang, Mette (Ekstern)
Main Supervisor:
Jensen, Peter Arendt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD

Systematic enzyme discovery, targeted to fungal and algal biomass

Department of Chemical and Biochemical Engineering
Combined flue gas cleaning for small scale wood combustion appliances

Department of Chemical and Biochemical Engineering
CHEC Research Centre
PHX innovation ApS
Period: 20/06/2016 → 19/06/2018
Number of participants: 2
Project participant:
Azizaddini, Seyednezamaddin (Intern)
Project Coordinator:
Illerup, Jytte Boll (Intern)

PhD position in Valorization of Industrial Waste Streams from Tuber Processing - Sino Danish Center (SDC)

Department of Chemical and Biochemical Engineering
Period: 01/06/2016 → 31/07/2019
Number of participants: 4
Phd Student:
Barrett, Kristian (Intern)
Supervisor:
Busk, Peter Kamp (Intern)
Meyer, Anne S. (Intern)
Main Supervisor:
Lange, Lene (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Thermodynamics, Design, Simulation and Benchmarking of Biofuel Processes

Department of Chemical and Biochemical Engineering
Period: 01/06/2016 → 31/05/2019
Number of participants: 3
Phd Student:
Torli, Mauro (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Fosbøl, Philip Loldrup (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Validation and Improvement of Property and Process Modelling for Oleochemicals
Department of Chemical and Biochemical Engineering
Period: 01/06/2016 → 31/05/2019
Number of participants: 5
Phd Student:
Forero-Hernandez, Hector Alexander (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Jensen, Anker Degn (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Sin, Gürkan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Enzymatic lignin biorefining by cleavage of lignin-carbohydrate complexes
Department of Chemical and Biochemical Engineering
Period: 15/05/2016 → 14/05/2019
Number of participants: 4
Phd Student:
Mosbech, Caroline (Intern)
Supervisor:
Wittrup Agger, Jane (Intern)
Busk, Peter Kamp (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Computational Fluid Dynamics (CFD) Study of Bio-Dust Combustion
Department of Chemical and Biochemical Engineering
Period: 01/05/2016 → 30/04/2019
Number of participants: 4
Phd Student:
Leth-Espensen, Anna (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Glarborg, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Heat Transfer in dielectric elastomers
Department of Chemical and Biochemical Engineering
Period: 01/05/2016 → 30/04/2019
Number of participants: 3
Phd Student:
Madsen, Line Riis (Intern)
Supervisor:
Hassager, Ole (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Surface Characterization of Activated Chalcopyrite Particles

Department of Chemical and Biochemical Engineering
Period: 01/05/2016 → 30/04/2019
Number of participants: 4
Phd Student:
Karcz, Adam Paul (Intern)
Supervisor:
Damør, Anne Juul (Intern)
Illerup, Jytte Boli (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Activities:
Materials Science and Technology 2016
Project: PhD

Thermodynamic modelling and data evaluation for life sciences applications

Department of Chemical and Biochemical Engineering
Period: 01/05/2016 → 30/04/2019
Number of participants: 4
Phd Student:
Ruszczynski, Lukasz (Intern)
Supervisor:
Sin, Gürkan (Intern)
Zubov, Alexandr (Intern)
Main Supervisor:
Abildskov, Jens (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Design and optimization of selected oleochemical processes

Department of Chemical and Biochemical Engineering
Period: 15/04/2016 → 14/04/2019
Number of participants: 4
Phd Student:
Jones, Mark Nicholas (Intern)
Supervisor:

Gernaey, Krist V. (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Sin, Gürkan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

In-silico Process Design and Evaluation Tool for Pharmaceutical Manufacturing

Department of Chemical and Biochemical Engineering
Period: 15/04/2016 → 14/04/2019
Number of participants: 3
Phd Student:
do Carmo Montes, Frederico da Conceicao (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Sin, Gürkan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Sustainable Process Synthesis and Design

Department of Chemical and Biochemical Engineering
Period: 15/04/2016 → 31/01/2017
Number of participants: 3
Phd Student:
Maria Dragan, Johanna (Intern)
Supervisor:
Zubov, Alexandr (Intern)
Main Supervisor:
Sin, Gürkan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Thermodynamics of Petroleum Fluids relevant to Subsea Processing

Department of Chemical and Biochemical Engineering
Period: 01/04/2016 → 31/03/2019
Number of participants: 3
Phd Student:
Kruger, Francois (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
von Solms, Nicolas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD
Fermentation of Synthesis Gas
Department of Chemical and Biochemical Engineering
Period: 01/03/2016 → 28/02/2019
Number of participants: 3
Phd Student:
Grimalt Alemany, Antonio (Intern)
Supervisor:
Skiadas, Ioannis V (Intern)
Main Supervisor:
Gavala, Hariklia N. (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Fermentation of Synthesis Gas and Design of Bioreactors
Department of Chemical and Biochemical Engineering
Period: 01/02/2016 → 31/01/2019
Number of participants: 3
Phd Student:
Asimakopoulos, Konstantinos (Intern)
Supervisor:
Gavala, Hariklia N. (Intern)
Main Supervisor:
Skiadas, Ioannis V (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Plantwide Monitoring and Control of Biochemical Processes
Department of Chemical and Biochemical Engineering
Period: 01/02/2016 → 31/10/2019
Number of participants: 3
Phd Student:
David Bähner, Franz (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Main Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Biomass Particle Morphology and Combustion Properties
Department of Chemical and Biochemical Engineering
Period: 01/01/2016 → 31/12/2018
Number of participants: 7
Phd Student:
Masche, Marvin (Intern)
Supervisor:
Puig Arnavat, Maria (Intern)
Clausen, Sønnik (Intern)
Henriksen, Ulrik Birk (Intern)
Holm, Jens Kai (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Ahrenfeldt, Jesper (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

**Biomass Particle ignition in mill equipment**
Department of Chemical and Biochemical Engineering
Period: 15/12/2015 → 14/01/2019
Number of participants: 5
Phd Student:
Schwarzer, Lars (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Glarborg, Peter (Intern)
Holm, Jens Kai (Intern)
Main Supervisor:
Jensen, Peter Arendt (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Energy production from seaweed and seaweed processing residues**
Department of Chemical and Biochemical Engineering
Period: 15/12/2015 → 04/03/2016
Number of participants: 3
Phd Student:
Iddrisu, Abdul-Mumeen (Ekstern)
Supervisor:
Thygesen, Anders (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

**Autosamling and monitoring of bioprocesses**
Department of Chemical and Biochemical Engineering
Period: 01/12/2015 → 07/01/2019
Number of participants: 4
Phd Student:
Pontius, Katrin (Intern)
Supervisor:
Junicke, Helena (Intern)
Hundebel, Ivan (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Development of Strategies for More Efficient CIP Cleaning

Department of Chemical and Biochemical Engineering
Period: 01/12/2015 → 30/11/2018
Number of participants: 3
Phd Student:
Yang, Jifeng (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Krühne, Ulrich (Intern)

Laccase engineering and reaction analysis

Department of Chemical and Biochemical Engineering
Period: 01/12/2015 → 30/11/2018
Number of participants: 3
Phd Student:
Perna, Valentina (Intern)
Supervisor:
Wittrup Agger, Jane (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Oxygen Blown Biomass Gasification

Department of Chemical and Biochemical Engineering
Period: 01/12/2015 → 30/11/2018
Number of participants: 5
Phd Student:
Ravenni, Giulia (Intern)
Supervisor:
Ahrenfeldt, Jesper (Intern)
Gebel, Benny (Intern)
Sárossy, Zsuzsa (Intern)
Main Supervisor:
Henriksen, Ulrik Birk (Intern)

Use of Ionic Liquids and Support Materials for High Performance Enzymatic Conversion of CO2 Into Formic Acid and Formaldehyde

Department of Chemical and Biochemical Engineering
Period: 01/12/2015 → 30/11/2018
Number of participants: 4
Phd Student: Zhang, Zhibo (Intern)
Supervisor: Zhang, Suo-Jiang (Ekstern)
von Solms, Nicolas (Intern)
Main Supervisor: Pinelo, Manuel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Thermodynamic property of ionic liquids/CO2 system and its applications: Highly efficient conversion of CO2 at mild conditions
Department of Chemical and Biochemical Engineering
Period: 15/11/2015 → 14/11/2018
Number of participants: 4
Phd Student: meng, Xianglei (Ekstern)
Supervisor: Liang, Xiaodong (Intern)
Zhang, Suo-Jiang (Ekstern)
von Solms, Nicolas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Silicone elastomers with aromatic voltage stabilizers
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Period: 01/11/2015 → 01/07/2016
Number of participants: 2
Aromatic voltage stabilizers, Silicone elastomers, Electron-trapping effect, PDMS-PPMS copolymers
Project ID: 52070
Project participant:
A Razak, Aliff Hisyam (Intern)
Skov, Anne Ladegaard (Intern)

Project
Advancing Modelling for Process-Product Innovation, Optimization, Monitoring and Control in Life Science Industries
Marie Skłodowska-Curie Actions
H2020-MSCA-ITN-2015 call
Grant agreement no.675251
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Alfa Laval
Imperial College London
University of Strathclyde
RWTH Aachen University
Bayer AG
Unilever
Universite Claude Bernard Lyon 1
Period: 01/11/2015 → 31/10/2019
Number of participants: 9
mathematical modeling, optimization, control, life sciences, biotechnology
Acronym: ModLife
Project ID: 675251
Number of related Ph.D. students: 5
Project Manager, organisational:
Zubov, Alexandr (Intern)
Phd Student:
Al, Resul (Intern)
Ruszczynski, Lukasz (Intern)
do Carmo Montes, Frederico da Conceicao (Intern)
Forero-Hernandez, Hector Alexander (Intern)
Jones, Mark Nicholas (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Project Coordinator:
Sin, Gürkan (Intern)

Design and Fabrication of Functionalized Ionic Liquid-based Polymeric Composite Membrane for CO2 Separation
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Period: 01/11/2015 → 31/10/2018
Number of participants: 5
Phd Student:
Song, Ting (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Zhang, Suo-Jiang (Ekstern)
Zhang, Xiangping (Ekstern)
Main Supervisor:
Szábo, Péter (Intern)

Financing sources
Source: Internal funding (public)
Design and Fabrication of Functionalized Ionic Liquid-based Polymeric Composite Membrane for CO2 Separation

Department of Chemical and Biochemical Engineering
Period: 01/11/2015 → 31/10/2018
Number of participants: 5
PhD Student:
Song, Ting (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Zhang, Suo-Jiang (Ekstern)
Zhang, Xiangping (Ekstern)
Main Supervisor:
Szabo, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Engineered yeast strains for the production of bulk chemicals from algae biomass

Novo Nordisk Foundation Center for Biosustainability
Applied Metabolic Engineering
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Period: 15/10/2015 → 14/10/2018
Number of participants: 3
Project participant:
Förster, Jochen (Intern)
Gernaey, Krist V. (Intern)
PhD Student:
Porcayo Loza, Javier (Intern)

Hydrogen assisted catalytic biomass pyrolysis for green fuels

Department of Chemical and Biochemical Engineering
Period: 01/10/2015 → 30/09/2018
Number of participants: 5
PhD Student:
Stummann, Magnus Zingler (Intern)
Supervisor:
Høj, Martin (Intern)
Jensen, Peter Arendt (Intern)
Sundet, Jostein K. (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Next Generation Methanol to Formamide Selective Oxidation Catalysts

Department of Chemical and Biochemical Engineering
Understanding Sulphuric Acid Accumulation in Lube oil in Diesel Engines
Department of Chemical and Biochemical Engineering
Period: 01/10/2015 → 30/09/2018
Number of participants: 4
Phd Student:
Lejre, Kasper Hartvig (Intern)
Supervisor:
Fosbøl, Philip Loldrup (Intern)
Glarborg, Peter (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Systematic computer aided methods and tools for lipids process technology
Department of Chemical and Biochemical Engineering
Period: 15/09/2015 → 14/09/2018
Number of participants: 5
Phd Student:
Ana Perederic, Olivia (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Kontogeorgis, Georgios (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Woodley, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Development of Large-Scale Processes Using Alcohol Oxidases
Department of Chemical and Biochemical Engineering
Period: 01/09/2015 → 31/10/2018
Number of participants: 3
Phd Student:
Dias Gomes, Mafalda (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Main Supervisor:
Woodley, John (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

**Estimation of Matrix Flow contribution in naturally fractured reservoirs**
Department of Chemical and Biochemical Engineering
Period: 01/09/2015 → 31/08/2018
Number of participants: 4
Phd Student: Brand Ferrell, Justin (Intern)
Supervisor: Stenby, Erling Halfdan (Intern)
Yan, Wei (Intern)
Main Supervisor: Shapiro, Alexander (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Privatist
Project: PhD

**Model based Biochemical Processes Monitoring**
Department of Chemical and Biochemical Engineering
Period: 01/09/2015 → 31/08/2018
Number of participants: 3
Phd Student: André Fernandes Caroço, Ricardo (Intern)
Supervisor: Abildskov, Jens (Ekstern)
Main Supervisor: Huusom, Jakob Kjøbsted (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

**Selective Catalytic Reduction of NOx from Ships**
Department of Chemical and Biochemical Engineering
Period: 01/09/2015 → 31/08/2018
Number of participants: 4
Phd Student: Christensen, Steen Müller (Intern)
Supervisor: Hansen, Brian Brun (Intern)
Pedersen, Kim Hougaard (Intern)
Main Supervisor: Jensen, Anker Degn (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD
Automating Experimentation in miniaturized reactors
Department of Chemical and Biochemical Engineering
Period: 15/08/2015 → 14/10/2018
Number of participants: 4
Phd Student:
Tajsoleiman, Tannaz (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Huusom, Jakob Kjøbsted (Intern)
Main Supervisor:
Krühne, Ulrich (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Bioprocess risk assessment using a mechanistic modelling framework
Department of Chemical and Biochemical Engineering
Period: 01/08/2015 → 31/07/2018
Number of participants: 4
Phd Student:
Spann, Robert (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Eliasson Lantz, Anna (Intern)
Main Supervisor:
Sin, Gürkan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Consistent Scale-up of the Freeze-drying Process
Department of Chemical and Biochemical Engineering
Period: 01/08/2015 → 31/07/2018
Number of participants: 5
Phd Student:
Teresa de Melo Machado Simoes Carvalho, Ana (Intern)
Supervisor:
Clausen, Anders (Intern)
Krühne, Ulrich (Intern)
Madsen, Michelle Milling (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt EU-finansieret
Project: PhD

Diabatic Separation of Fermentation Liquids
Department of Chemical and Biochemical Engineering
Period: 01/08/2015 → 30/04/2017
Number of participants: 3
Phd Student:
Jesper Greisen Larsen, Morten (Intern)
**Low friction non-fouling coatings for high fuel efficiency at reduced speed**

Department of Chemical and Biochemical Engineering  
Period: 01/08/2015 → 31/07/2018  
Number of participants: 4  
PhD Student:  
Wang, Xueting (Intern)  
Supervisor:  
Dam-Johansen, Kim (Intern)  
Tullberg, Marcus (Ekstern)  
Main Supervisor:  
Kiil, Søren (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansieret - Andet  
Project: PhD

**Thermochemical Conversion of Biomass**

Department of Chemical and Biochemical Engineering  
Period: 01/08/2015 → 31/07/2018  
Number of participants: 4  
PhD Student:  
Anicic, Bozidar (Intern)  
Supervisor:  
Lin, Weigang (Intern)  
Wu, Hao (Intern)  
Main Supervisor:  
Dam-Johansen, Kim (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Offentlig finansiering  
Project: PhD

**Development of large-scale processes for baeyer-Villiger Biocatalysis**

Department of Chemical and Biochemical Engineering  
Period: 15/07/2015 → 14/07/2018  
Number of participants: 3  
PhD Student:  
Meissner, Murray Peter (Intern)  
Supervisor:  
Krühne, Ulrich (Intern)  
Main Supervisor:  
Woodley, John (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Anden EU-finansiering  
Project: PhD
Thermodynamics, Design, Simulation and Benchmarking of Biofuel Processes
A new framework at DTU contributes to the sustainable development of technologies for green synthetic fuel production from biomass. Thermochemical biomass gasification is carried out, followed by fermentation of the created syngas to biofuels. The ultimate scope is a complete design which will include energy efficient product separation, process analysis and optimization as well as comparison to competitive market Technologies.

In brief, the technological focus and scientific objectives are: 1) Fermentation of syngas to liquid (alcohols) and gaseous (methane) biofuels focusing on applying mixed microbial consortia, 2) Design of novel bioreactors, pressure control and use of suitable surfactants for increasing the gas/liquid mass transfer efficiency, 3) Use of biomimetic membranes and development of diabatic distillation for gentle and cost-efficient purification of liquid biofuels and 4) Development of an optimized process design and comparison with existing Technologies.

The technology to be developed will contribute to a more sustainable society producing energy from non-food related biomass without a catalytic conversion. Today syngas from biomass is used in combined heat and power production (CHP). By merging the CHP production with the fermentation of syngas, the processing of syngas can always follow the optimum path. That is, the final production will be easily diverted to CHP or biofuels satisfying thus the supply and demand of the biomass and energy markets. For example, when the heating demand is high, the syngas will mainly be exploited through CHP but when the heating demand is low, the syngas will be fermented to storable liquid or gaseous biofuels.

Purpose of the project

The task is to process simulate the fermentation technologies of syngas developed in this project. This covers both methanation and liquid fuel production. Simulations will be carried out and compared to other competitive literature methods to benchmark the technologies from a mass, energy, economic and engineering point of view. The designs will likely be carried out with the commercial process simulator Aspen Plus.

Project contents

The core of your project is to develop a thermodynamic model parameter base. Knowledge will be collected from the project platform to model the observed phenomenon. The investigations will include data from literature and includes thermodynamic modeling, possibly supported by experimental work. The knowledge will be applied in software programming and in a more high level process simulation interface to Aspen Plus. The CERE group has a selection of available interfaces which will be exploited as part of this work. The global aim is to perform process simulation of several different syngas fermentation designs and furthermore compare these with the aim of benchmarking the performance of the various technologies towards commercial processes.

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering

CERE – Center for Energy Resources Engineering
Period: 01/07/2015 → 30/06/2019
Number of participants: 1
Acronym: Synferon
Project participant:
Fosbøl, Philip Loldrup (Intern)

Sulphur (SOx) corrosion in large diesel engines

Project entails experimental and modeling of current densities during corrosion from sulphur as a consequence of the combustion process in large diesel ship engines

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering

CERE – Center for Energy Resources Engineering
Period: 01/07/2015 → 01/01/2019
Number of participants: 1
Acronym: SulCor
Number of related Ph.D. students: 1
**Sulcor - Securing Corrosion Free Conditions**

Department of Chemical and Biochemical Engineering  
Period: 01/07/2015 → 30/06/2018  
Number of participants: 5  
Phd Student:  
Nielsen, Henrik Lund (Intern)  
Supervisor:  
Glarborg, Peter (Intern)  
Kiil, Søren (Intern)  
Thomsen, Kaj (Intern)  
Main Supervisor:  
Fosbøl, Philip Loldrup (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansieret - Andet  
Project: PhD

**Application of forward osmosis for water recovery and effluent up-concentration: the case of fermentative butanol production from crude glycerol**

Department of Chemical and Biochemical Engineering  
Period: 01/06/2015 → 30/09/2017  
Number of participants: 6  
Phd Student:  
Kalafatakis, Stavros (Intern)  
Supervisor:  
Skiadas, Ioannis V (Intern)  
Main Supervisor:  
Gavala, Hariklia N. (Intern)  
Examiner:  
Pinelo, Manuel (Intern)  
Christensen, Morten Lykkegaard (Ekstern)  
Venus, Joachim (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansieret - Andet  
Project: PhD

**Aqueous Ammonia Soaking as a pretreatment of lignocellulosic biomasses for improving manurebafor enhancing biogas yield from lignocellulosic biomasses sed anaerobiv digestion**

Department of Chemical and Biochemical Engineering  
Period: 01/06/2015 → 13/11/2017  
Number of participants: 6  
Phd Student:  
Lymperatou, Anna (Intern)  
Supervisor:  
Gavala, Hariklia N. (Intern)  
Main Supervisor:  
Skiadas, Ioannis V (Intern)  
Examiner:  
Pinelo, Manuel (Intern)  
Carrere, Hélène (Ekstern)
Holm-Nielsen, Jens Bo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Durable Zeolite Based Catalyst Systems for Diesel Emission Control
Department of Chemical and Biochemical Engineering
Period: 15/05/2015 → 14/05/2018
Number of participants: 3
Phd Student:
Hammershøi, Peter Sams (Intern)
Supervisor:
Janssens, Ton V. W. (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD

HCl emission from cement plants
Department of Chemical and Biochemical Engineering
Period: 15/05/2015 → 14/05/2018
Number of participants: 5
Phd Student:
Pachitsas, Stylianos (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Jensen, Lars Skaarup (Intern)
Jensen, Lars Skaarup (Intern)
Main Supervisor:
Wedel, Stig (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Multiphase flow and fuel conversion in cement calciner
Department of Chemical and Biochemical Engineering
Period: 15/05/2015 → 11/08/2018
Number of participants: 6
Phd Student:
Nakhaei, Mohammadhadi (Intern)
Supervisor:
Glarborg, Peter (Intern)
Grevain, Damien (Ekstern)
Jensen, Lars Skaarup (Intern)
Wu, Hao (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
**Application of an association equation of state to enhanced oil recovery processes**

Department of Chemical and Biochemical Engineering  
Period: 01/05/2015 → 30/06/2018  
Number of participants: 3  
Phd Student: Pinto Coelho Muniz Vinhal, Andre (Intern)  
Supervisor: Yan, Wei (Intern)  
Main Supervisor: Kontogeorgis, Georgios (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Science Without Borders, Brasi  
Project: PhD

**The implementation of anammox in a full-scale industrial waste-water treatment plant**

Department of Chemical and Biochemical Engineering  
Period: 01/04/2015 → 31/07/2018  
Number of participants: 4  
Phd Student: Feldman, Hannah (Intern)  
Supervisor: Flores Alsina, Xavier (Intern)  
Main Supervisor: Sin, Gürkan (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansierede - Virksomhed  
Project: PhD

**Anti-stick coatings in the cement and mineral industries**

Department of Chemical and Biochemical Engineering  
Period: 01/03/2015 → 31/08/2016  
Number of participants: 4  
Phd Student: Mørk, Kasper Skov (Intern)  
Supervisor: Dam-Johansen, Kim (Intern)  
Main Supervisor: Sivebæk, Ion Marius (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansierede - Virksomhed  
Project: PhD

**Burners for Cement Kilns**

Department of Chemical and Biochemical Engineering  
Period: 01/03/2015 → 30/04/2018  
Number of participants: 4  
Phd Student:
Pedersen, Morten Nedergaard (Intern)
Supervisor:
Clausen, Sønnik (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)

Financial sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Modeling of gradients in large scale bioreactors
Department of Chemical and Biochemical Engineering
Period: 01/03/2015 → 12/04/2018
Number of participants: 6
Phd Student:
Bach, Christian (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Woodley, John (Intern)
Nordkvist, Mikkel (Intern)
Takors, Ralf (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Fractionation and enzymatic processing of biomass for biorefinery applications
Department of Chemical and Biochemical Engineering
Period: 01/02/2015 → 30/04/2018
Number of participants: 4
Phd Student:
Tristan Djajadi, Demi (Intern)
Supervisor:
Jørgensen, Henning (Intern)
Pinelo, Manuel (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Financial sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Study of Fixed Film Fixed Filter AD (4FAD) Biogas System Performance at High Suspende Solids and COD loads
Department of Chemical and Biochemical Engineering
Period: 01/02/2015 → 31/01/2019
Number of participants: 5
Phd Student:
Gonzalez Londono, Jorge Enrique (Intern)
Supervisor:
Jensen, Anders Peter (Ekstern)
Thomsen, Kaj (Intern)
Uller, Bjarne (Eksternt)
Main Supervisor:
Meyer, Anne S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Seaweed Biorefinery in Ghana
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 01/01/2015 → 30/06/2017
Number of participants: 1
Acronym: SeaBioGha
Supervisor:
Ale, Marcel Tutor (Intern)

Relations
Activities:
Seaweed Biorefinery in Ghana (SeaBioGha) (External organisation)
Presentation for Seaweed Biorefinery in Ghana (SeaBioGha) - Danida funded project (External organisation)

Publications:
Functional hydrocolloids from seaweeds
Project

Catalysis Methanol Synthesis
Department of Chemical and Biochemical Engineering
Period: 01/01/2015 → 31/05/2016
Number of participants: 5
Phd Student:
Liu, Yawen (Intern)
Supervisor:
Christensen, Jakob Munkholt (Intern)
Dam-Johansen, Kim (Intern)
Lin, Weigang (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Cellulase enzymology and production
Department of Chemical and Biochemical Engineering
Period: 01/01/2015 → 31/12/2017
Number of participants: 8
Phd Student:
Bentil, Joseph Asankomah (Intern)
Supervisor:
Lange, Lene (Intern)
Thygesen, Anders (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Enzyme discovery for seaweed processing

Department of Chemical and Biochemical Engineering
Period: 01/01/2015 → 16/04/2018
Number of participants: 4
Phd Student:
Cao, Thi Thuy Hang (Intern)
Supervisor:
Dalgaard Mikkelsen, Maria (Intern)
Mikkelsen, Jørn Dalgaard (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Research of conductive spinning solution in ionic liquid and enzymatic modification cellulose system

Department of Chemical and Biochemical Engineering
Period: 01/01/2015 → 31/12/2017
Number of participants: 7
Phd Student:
Liu, Yanrong (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Zhang, Suo-Jiang (Ekstern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
von Solms, Nicolas (Intern)
Chiappe, Cinzia (Ekstern)
Guo, Zheng (Intern)

Development of Optimal Operating Conditions for Producing Single Cell Protein

Department of Chemical and Biochemical Engineering
Period: 15/12/2014 → 15/09/2018
Number of participants: 4
Phd Student:
Wu, Mengzhe (Intern)
Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Krühne, Ulrich (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

NOx reduction in grate-firing solid waste power plants
Department of Chemical and Biochemical Engineering
Period: 15/12/2014 → 14/12/2017
Number of participants: 7
Phd Student:
Jepsen, Morten Søe (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Norman, Thomas (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Hvid, Søren Lovmand (Ekstern)
Løvås, Terese (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD

Investigation of oxygen-blown biomass gasification
Department of Chemical and Biochemical Engineering
Period: 01/12/2014 → 21/06/2018
Number of participants: 4
Phd Student:
Gadsbøll, Rasmus Østergaard (Intern)
Supervisor:
Ahrenfeldt, Jesper (Intern)
Clausen, Lasse Røngaard (Intern)
Main Supervisor:
Henriksen, Ulrik Birk (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Seaweed polysaccharides production using enzymes technologies
Department of Chemical and Biochemical Engineering
Period: 01/12/2014 → 16/12/2017
Number of participants: 7
Phd Student:
Rhein-Knudsen, Nanna (Intern)
Supervisor:
Holck, Jesper (Intern)
Dalgaard Mikkelsen, Maria (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Optimal Model Based Process Monitoring of Tubular Reactors

Department of Chemical and Biochemical Engineering
Period: 15/11/2014 → 14/05/2018
Number of participants: 4
Phd Student:
Ramirez Castelan, Carlos Eduardo (Intern)
Supervisor:
Brix, Jacob (Intern)
Jensen, Anker Degn (Intern)
Main Supervisor:
Huusom, Jakob Kjøbsted (Intern)

Catalytic Hydro-Liquefaction of Lignin to Value added Chemicals

Department of Chemical and Biochemical Engineering
Period: 01/11/2014 → 30/04/2018
Number of participants: 4
Phd Student:
Ghafarnejad Parto, Soheila (Intern)
Supervisor:
Christensen, Jakob (Ekstern)
Taarning, Esben (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

PSMsolubilization of inorganic phosphorus in gasified waste products: optimization of the performance and persistence of biofertilizers in different soil/crop systems

Department of Chemical and Biochemical Engineering
Period: 01/11/2014 → 31/12/2014
Number of participants: 4
Phd Student:
Raymond, Nelly (Ekstern)
Supervisor:
Hauggaard-Nielsen, Henrik (Intern)
Müller-Stöver, Dorette Sophie (Intern)
Main Supervisor:
Pilegaard, Kim (Intern)
Prediction of Deposit Formation in Biomass Fired Suspension Boilers - Gaining fundamental Data needed for Mechanistic Deposit Modelling

Department of Chemical and Biochemical Engineering
Period: 15/10/2014 → 14/10/2017
Number of participants: 8
Phd Student:
Laxminarayan, Yashasvi (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Giarborg, Peter (Intern)
Giarborg, Peter (Intern)
Main Supervisor: Jensen, Peter Arendt (Intern)
Examiner:
Wedel, Stig (Ekstern)
Hupa, Mikko (Ekstern)
Norman, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Characterization of Microbial consortia for keratin degradation processes

Department of Chemical and Biochemical Engineering
Period: 01/10/2014 → 30/04/2018
Number of participants: 3
Phd Student:
Falco, Francesco Cristino (Intern)
Supervisor:
Eliasson Lantz, Anna (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Sustainable process design with process intensification

Department of Chemical and Biochemical Engineering
Period: 01/10/2014 → 14/02/2018
Number of participants: 6
Phd Student:
Frauzem, Rebecca (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Bode, Andreas (Ekstern)
Zondervan, Edwin (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Publications:
Sustainable process design with process intensification - Development and implementation of a framework for sustainable carbon dioxide capture and utilization processes
Project: PhD

Using Coal Ash and other Additives in Suspension Fired Biomass Power Plant Boilers using Coal Ash and other Additives in Suspension Fired Biomass Power plant Boilers
Department of Chemical and Biochemical Engineering
Period: 01/10/2014 → 28/02/2018
Number of participants: 9
Phd Student:
Wang, Guoliang (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Glarborg, Peter (Intern)
Glarborg, Peter (Intern)
Wu, Hao (Intern)
Main Supervisor:
Jensen, Peter Arendt (Intern)
Examiner:
Lin, Weigang (Intern)
Pettersson, Anita (Ekstern)
Wadenbäck, Johan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Computer-aided Mixture and Blend Design
Department of Chemical and Biochemical Engineering
Period: 15/09/2014 → 24/01/2018
Number of participants: 7
Phd Student:
Cignitti, Stefano (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Gernaey, Krist V. (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Camarda, Kyle V. (Ekstern)
Kate, Antoon J. B. ten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Optimization-based design of waste heat recovery systems
Project: PhD
Continuous crystallization and filtration of Ective Pharmaceutical Ingredients and Intermediates for pharmaceutical production

Department of Chemical and Biochemical Engineering
Period: 15/09/2014 → 24/11/2017
Number of participants: 8
Phd Student:
Capellades Mendez, Gerard (Intern)
Supervisor:
Christensen, Troels V. (Ekstern)
Dam-Johansen, Kim (Intern)
Mealy, Michael J. (Ekstern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Glennon, Brian (Ekstern)
Lopez de Diego, Heidi (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed

Relations
Publications:
Design of Continuous Crystallizers for Production of Active Pharmaceutical Ingredients
Project: PhD

On the correlation between Young’s modulus and melt flow in fiber spinning operations

Department of Chemical and Biochemical Engineering
Period: 15/09/2014 → 13/11/2017
Number of participants: 6
Phd Student:
Wingstrand, Sara Lindeblad (Intern)
Supervisor:
Szabo, Peter (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Skov, Anne Ladegaard (Intern)
Peters, Gerrit W.M. (Ekstern)
von Ruymbeke, Evelyne (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed

Relations
Publications:
On the link between nonlinear extensional rheology and morphology of polymeric fibers
Project: PhD

Modelling, Synthesis and Analysis of Biorefinery Networks

Department of Chemical and Biochemical Engineering
Period: 01/09/2014 → 14/02/2018
Number of participants: 7
Phd Student:
Bertran, Maria-Ona (Intern)
Model-based interpretation of microbioreactor data

Department of Chemical and Biochemical Engineering
Period: 15/08/2014 → 15/02/2018
Number of participants: 7
PhD Student:
Semenova, Daria (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Marty, Jean Louis (Ekstern)
Santos, David Hernández (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Protective Coatings in the Cement and Mineral Industry

Department of Chemical and Biochemical Engineering
Period: 15/08/2014 → 14/03/2018
Number of participants: 7
PhD Student:
Møller, Victor Buhl (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Abildskov, Jens (Ekstern)
Paulsen, Andreas Lundtang (Intern)
Paulsen, Andreas Lundtang (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD
Temperature and poroelasticity of sedimentary rocks

The project is centered on development of rock mechanics related to high pressure and high temperature (HP/HT) conditions in the subsurface. The issue will be addressed experimentally and theoretically including numerical modeling.

Hydrocarbon reservoirs deeply buried under the central North Sea are not only subjected to high temperatures and a stress-field corresponding to depths of 5 km or more. They are also situated at a depth with high regional overpressure. This gives rise to three key challenges, which apply not only in the North Sea but world-wide: 1. Safety during drilling operations due to the extreme pressure and stresses. 2. Well life – the danger of well collapse under extreme stress conditions. 3. Controlling the drilling operation due to narrow drilling windows, in particular during infill drilling. This latter challenge must be met in order to maximize recovery.

In order to address these challenges we must develop methods to determine how the effective stress field responds to changes in pore pressure under these extreme conditions. The effective stress field is primarily a function of the weight of the overburden and how much of the load, the fluids in the rock carry. It also depends on the elastic properties of the rock at a given depth.

Supervisor: Prof. Ida Lykke Fabricius, ilfa@byg.dtu.dk
co-supervisor: Ass. Prof. Katrine Alling Andreassen, kall@byg.dtu.dk

Department of Civil Engineering
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Department of Geology and Geotechnical Engineering

Period: 01/08/2014 → 01/08/2017
Number of participants: 1
Project participant:
Orlander, Tobias (Intern)

Relations
Related projects:
Heat Storage in Hot Aquifers

Fractionation and processing of biomass for biorefinery applications

Department of Chemical and Biochemical Engineering

Period: 01/08/2014 → 14/10/2014
Number of participants: 3
Phd Student:
Maimann, Michael (Intern)
Supervisor:
Pinelo, Manuel (Intern)
Main Supervisor:
Jørgensen, Henning (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Modification of polymer surfaces to enhance enzyme activity and stability

Department of Chemical and Biochemical Engineering

Period: 01/08/2014 → 13/12/2017
Number of participants: 7
Phd Student:
Hoffmann, Christian (Intern)
Supervisor:
Pinelo, Manuel (Intern)
Woodley, John (Intern)
Main Supervisor:
Daugaard, Anders Egede (Intern)
Examiner:
Szabo, Peter (Intern)
Gardossi, Lucia (Ekstern)
Malkoch, Michael (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Publications:
Modification of polymer surfaces to enhance enzyme activity and stability
Project: PhD

Micro Scale Reactor System development with integrated advanced sensor technology
Department of Chemical and Biochemical Engineering
Period: 01/07/2014 → 24/01/2018
Number of participants: 6
Phd Student:
Oliveira Fernandes, Ana Carolina (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Krühne, Ulrich (Intern)
Examiner:
Eliasson Lantz, Anna (Intern)
Kockmann, Norbert (Ekstern)
Wohlgemuth, Roland (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)

Relations
Publications:
Micro scale reactor system development with integrated advanced sensor technology: A modular approach to the development of microfluidic screening platforms
Project: PhD

Computer-aided molecular design of novel working fluids to optimize heat transfer processes
Department of Chemical and Biochemical Engineering
Period: 01/06/2014 → 25/08/2017
Number of participants: 6
Phd Student:
Frutiger, Jerome (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
von Solms, Nicolas (Intern)
Bode, Andreas (Ekstern)
Papadopoulos, Athanasios (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations

Publications:
Property Uncertainty Analysis and Methods for Optimal Working Fluids of Thermodynamic Cycles
Project: PhD

Development of the Electrolyte CPA Equation of State
Department of Chemical and Biochemical Engineering
Period: 01/06/2014 → 20/05/2018
Number of participants: 6
Phd Student:
Schlaikjer, Anders Tviis (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Woodley, John (Intern)
Georgiadis, Michael C. (Ekstern)
Mujtaba, Iqbal M. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

New Catalysts for Emissions Reduction in diesel Engines
Department of Chemical and Biochemical Engineering
Period: 01/06/2014 → 31/03/2018
Number of participants: 2
Phd Student:
Allen, Ian (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

New fungal endomannanase diversity for mannan containing substrates in bioenergy
Department of Chemical and Biochemical Engineering
Period: 01/06/2014 → 07/07/2018
Number of participants: 4
Phd Student:
von Freiesleben, Pernille (Intern)
Supervisor:
Jørgensen, Henning (Intern)
Krogh, Kristian Bertel Rømer (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD
Integration between enzyme technology and membrane separation in biorefinery processes

Department of Chemical and Biochemical Engineering
Period: 01/05/2014 → 25/08/2017
Number of participants: 6
Phd Student:
Morthensen, Sofie Thage (Intern)
Supervisor:
Meyer, Anne S. (Intern)
Main Supervisor:
Pinelo, Manuel (Intern)
Examiner:
Hélix-Nielsen, Claus (Intern)
Christensen, Morten Lykkegaard (Ekstern)
Wallberg, Ola (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

PSM-solubilization of inorganic phosphorus in gasified waste products: molecular mechanisms and role of AMF in P transfer to plants

Department of Chemical and Biochemical Engineering
Period: 01/05/2014 → 31/12/2014
Number of participants: 4
Phd Student:
Efthymiou, Aikaterini (Intern)
Supervisor:
Grønlund, Mette (Intern)
Pilegaard, Kim (Intern)
Main Supervisor:
Jakobsen, Iver (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Biooxidation reactor and process design

Department of Chemical and Biochemical Engineering
Period: 01/04/2014 → 13/11/2017
Number of participants: 6
Phd Student:
Pedersen, Asbjørn Toftgaard (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Meyer, Anne S. (Intern)
Hauer, Bernhard (Ekstern)
Schmid, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
New catalysts for hydrodeoxygenation of biomass pyrolysis oil

Department of Chemical and Biochemical Engineering
Period: 01/04/2014 → 31/12/2017
Number of participants: 8
Phd Student:
Dabros, Trine Marie Hartmann (Intern)
Supervisor:
Gabrielsen, Jostein (Intern)
Grunwaldt, Jan-Dierk (Intern)
Høj, Martin (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Christensen, Jakob Munkholt (Intern)
Østberg, Martin (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Advanced thermodynamic cycles utilising low-temperature heat sources

Energy sources at a low temperature level are available from a variety of sources ranging from waste heat from ships, industry and refrigeration plants, to renewable energy in the form of biomass, geothermal and solar.

There is significant potential for improving the use of these sources in developing new cycles based on new multi-component fluid mixtures. These improvements will not only increase the efficiency of today’s technology, but they will also make it possible to use low-temperature sources which, due to lack of technical feasibility or economy is not used today. This ambitious, interdisciplinary project will lead the way to innovative thermal system for electricity generation, heat pumping and cooling by utilization of low value sources, at efficiencies that surpasses today’s level significantly. The project will develop advances in the design of both processes and media so that energy savings of 15% can be achieved. The analysis will include numerical simulation and advanced thermodynamic methods based on energy and exergy analysis and experimental verification of component performance. The development of a systematic approach to the optimization of cycle and the working medium in the given application. The results will provide a scientific basis for choosing the future use of low-temperature resources in Denmark. This may contribute significantly to the development of the future society using no fossil resources, but large amounts of fluctuating renewable energy.

Department of Mechanical Engineering

Thermal Energy
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Danish Technological Institute
Danfoss A/S
Viegand Maagæe
Alfa Laval
MAN Diesel & Turbo SE
A. P. Møller-Mærsk
Arla Foods
Technical University of Munich  
Delft University of Technology  
Aalborg University  
Alfa Laval  
Period: 01/03/2014 → 28/02/2019  
Number of participants: 17  
Acronym: THERMCYC  
Project ID: 76567  
Number of related Ph.D. students: 7  
Project participant:  
Haglind, Fredrik (Intern)  
Clausen, Lasse Røngaard (Intern)  
Kaer, Martin Ryhl (Intern)  
Markussen, Wiebke Brix (Intern)  
Sin, Gürkan (Intern)  
Gani, Rafiqul (Intern)  
Babi, Deenesh Kavi (Intern)  
Pierobon, Leonardo (Intern)  
Zhang, Lei (Intern)  
Zühlsdorf, Benjamin (Intern)  
Mancini, Roberta (Intern)  
Phd Student:  
Meroni, Andrea (Intern)  
Andreasen, Jesper Graa (Intern)  
Cignitti, Stefano (Intern)  
Frutiger, Jerome (Intern)  
Project Manager, academic:  
Elmegaard, Brian (Intern)  
Project Coordinator:  
Sørensen, Iben (Intern)  

Relations  
Activities:  
International Workshop on High Temperature Heat Pumps  
Publications:  
Book of presentations of the International Workshop on High Temperature Heat Pumps  
Mapping of low temperature heat sources in Denmark  
Improving efficiency of heat pumps by use of zeotropic mixtures for different temperature glides  
High Temperature Heat Pump Integration using Zeotropic Working Fluids for Spray Drying Facilities  
Derivation of guidelines for the design of plate evaporators in heat pumps using zeotropic mixtures  
Forbedring af industrielle processers energieffektivitet  
Project report: Experimental planning and verification of working fluids (WP 5)  
Industrial Energy Mapping: THERMCYC WP6  
Project

enzyme-enhanced CO2 Absorption - rate-based modeling and pilot-scale validation

Department of Chemical and Biochemical Engineering  
Period: 01/03/2014 → 25/08/2017  
Number of participants: 7  
Phd Student:  
Gladis, Arne Berthold (Intern)  
Supervisor:  
Fosbøl, Philip Loldrup (Intern)  
Woodley, John (Intern)  
Main Supervisor:  

Biorefining of hemp seeds: Enzymatic assisted upgrading technology
Optimize the extraction conditions of hemp seed protein using different enzyme preparations. To evaluate statistically the effect of different defatting techniques on amino acid quality and quantity of hemp protein isolates (HPI). To study different cellular structure and composition [e.g. Protein, amino acid (e.g. cysteine and methionine) and carbohydrates] of different plant seed materials. To explore different extraction methods (experimental and industrial scale) for the production of protein from different plant seed materials.

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 17/02/2014 → 18/07/2014
Number of participants: 3
Project participant:
Pinelo, Manuel (Intern)
Supervisor:
Meyer, Anne S. (Intern)
Main Supervisor:
Ale, Marcel Tutor (Intern)

Relations
Parent project:
Extraction of protein and amino acid from hemp seed meal
Project

Chemical Bioreaction Engineering methods for Plant Seed Upgrading: Literature review and introductory experimental work
To study different cellular structure and composition (e.g. Protein, amino acid and carbohydrates) of different plant seed materials. To explore different extraction methods (experimental and industrial scale) for the production of protein from different plant seed materials.

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 06/01/2014 → 24/01/2014
Number of participants: 3
Project participant:
Pinelo, Manuel (Intern)
Supervisor:
Meyer, Anne S. (Intern)
Main Supervisor:
Ale, Marcel Tutor (Intern)

Relations
Parent project:
Extraction of protein and amino acid from hemp seed meal
Related projects:
Characterization and production of protein isolates from oil-cold-pressed hemp seed meal
Enhancement of dielectric permittivity by incorporating PDMS-PEG multiblock copolymers in silicone elastomers

A silicone elastomer from PDMS-PEG multiblock copolymer has been prepared by use of silylation reactions for both copolymer preparation and crosslinking. The dielectric and mechanical properties of the silicone elastomers were carefully investigated, as well as the morphology of the elastomers was investigated by SEM. The developed silicone elastomers were too conductive to be utilized as dielectric elastomers but it was shown that when the above silicone elastomers were mixed with a commercial silicone elastomer, the resulting elastomer had very favourable properties for dielectric elastomers due to a significantly increased dielectric permittivity. The conductivity also remained low due to the resulting discontinuity in PEG within the silicone matrix.

Department of Chemical and Biochemical Engineering

The Danish Polymer Centre
Period: 01/01/2014 → 31/12/2014
Number of participants: 3
PDMS-PEG block copolymers, high permittivity, silicone elastomers, hydrosilylation
Project ID: 52070
Project participant:
A Razak, Aliff Hisyam (Intern)
Szabo, Peter (Intern)
Project Coordinator:
Skov, Anne Ladegaard (Intern)

Modeling of Asphaltene systems with Association Models

Department of Chemical and Biochemical Engineering
Period: 01/01/2014 → 26/04/2017
Number of participants: 6
Phd Student:
Arya, Alay (Intern)
Supervisor:
von Solms, Nicolas (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Yan, Wei (Intern)
Serensen, Henrik (Ekstern)
Vargas, Francisco M. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Continuous crystallization and filtration in production of pharmaceuticals

Department of Chemical and Biochemical Engineering
Period: 15/12/2013 → 07/02/2014
Number of participants: 3
Phd Student:
Visan, Aura (Ekstern)
Supervisor:
Dam-Johansen, Kim (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD
Developments in enzyme immobilization with downstream renewable energy applications
Department of Chemical and Biochemical Engineering
Period: 15/12/2013 → 25/08/2017
Number of participants: 6
Phd Student: Mohd Sueb, Mohd Shafiq Bin (Intern)
Supervisor: Meyer, Anne S. (Intern)
Main Supervisor: Pinelo, Manuel (Intern)
Examiner: Gavala, Hariklia N. (Intern)
Kádár, Zsófia (Intern)
Kroff, Pablo (Intern)

Financial sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Fluid dynamics and reactions in high-temperature gas-solid Energy Processes
Department of Chemical and Biochemical Engineering
Period: 15/12/2013 → 31/01/2017
Number of participants: 6
Phd Student: Ahli Gharamaleki, Mohammad (Intern)
Supervisor: Lin, Weigang (Intern)
Main Supervisor: Dam-Johansen, Kim (Intern)
Examiner: Jensen, Anker Degn (Intern)
Jensen, Bjarne Henning (Ekstern)
Song, Wenli (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Improved LCA Methodology and software tool for biorenewable products and processes
Department of Chemical and Biochemical Engineering
Period: 15/12/2013 → 25/01/2017
Number of participants: 6
Phd Student: Kumar Tula, Anjan (Intern)
Supervisor: Huusom, Jakob Kjøbsted (Intern)
Main Supervisor: Gani, Rafiqul (Intern)
Examiner: Woodley, John (Intern)
Harper, Peter Mathias (Intern)
Manenti, Flavio (Ekstern)

Financial sources
Relations
Publications:
Computer-Aided Sustainable Process Synthesis-Design and Analysis
Project: PhD

Production of prebiotic oligosaccharides by biocatalysis
Department of Chemical and Biochemical Engineering
Period: 15/12/2013 → 13/11/2017
Number of participants: 7
Phd Student:
Binti Jamek, Shariza (Intern)
Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Muschiol, Jan (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Lange, Lene (Intern)
Christensen, Morten Würtz (Ekstern)
Vaaje-Kolstad, Gustav (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

A chemical approach to avoiding electromechanical instabilities in dielectric electroactive polymer films
Department of Chemical and Biochemical Engineering
Period: 01/12/2013 → 15/05/2017
Number of participants: 6
Phd Student:
A Razak, Aliff Hisyam (Intern)
Supervisor:
Szabo, Peter (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Carpi, Federico (Ekstern)
Sommer-Larsen, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet

Relations
Publications:
Optimisation of Silicone-based Dielectric Elastomer Transducers by Means of Block Copolymers - Synthesis and Compounding
Project: PhD

Design of hydrophilic polymers for activated non-fouling coatings
Department of Chemical and Biochemical Engineering
Period: 01/12/2013 → 15/03/2017
Number of participants: 8
Development og highly efficient solid oxide electrolyzer cell systems

Department of Chemical and Biochemical Engineering
Period: 01/12/2013 → 30/09/2017
Number of participants: 7
PhD Student:
Duhn, Jakob Dragstæk (Intern)
Supervisor:
Wedel, Stig (Ekstern)
Wix, Christian (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Jensen, Søren Højgaard (Intern)
Deutschmann, Olaf (Ekstern)
Mortensen, Peter Mølgaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD

Relations
Publications:
Development of highly efficient solid oxide electrolyzer cell systems
Project: PhD
Eliasson Lantz, Anna (Intern)
Adlercreutz, Patrick (Ekstern)
Meurer, Guido (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering

Relations
Publications:
Benchmarking of Processes for the Biosynthesis of Natural Products
Project: PhD

HP/HT reservoir fluids with focus on scaling and thermo

Department of Chemical and Biochemical Engineering
Period: 01/12/2013 → 23/05/2018
Number of participants: 3
Phd Student:
Figueroa Murcia, Diana Carolina (Intern)
Supervisor:
Fosbøl, Philip Loldrup (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Novel Strategies for Fermentation Control

Department of Chemical and Biochemical Engineering
Period: 01/12/2013 → 15/03/2017
Number of participants: 8
Phd Student:
Mears, Lisa (Intern)
Supervisor:
Sin, Gürkan (Intern)

Stocks, Stuart M. (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Huusom, Jakob Kjebsted (Intern)
Glassey, Jarmila (Ekstern)
Kold, David (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed

Relations
Publications:
Novel strategies for control of fermentation processes
Project: PhD

Predictive modeling of gas diffusion and solubility in polymers for offshore pipelines

Department of Chemical and Biochemical Engineering
Investigation of Aspergillus niger aggregation behaviour and its relationship to industrial fermentation
Department of Chemical and Biochemical Engineering
Period: 15/11/2013 → 08/08/2018
Number of participants: 4
PhD Student:
Hagemann, Timo (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Structural characterization and enzymatic modification of soy polysaccharides
Department of Chemical and Biochemical Engineering
Period: 15/11/2013 → 25/08/2017
Number of participants: 7
PhD Student:
Pierce, Brian (Intern)
Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Wichmann, Jesper (Ekstern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Pinelo, Manuel (Intern)
Kabel, Mirjam Anna (Ekstern)
Pedersen, Lars Hastrup (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD

Relations
Publications:
Structural Characterization and Enzymatic Modification of Soybean Polysaccharides
Project: PhD
Sustainable design of biorefinery systems for biorenewables

Department of Chemical and Biochemical Engineering
Period: 15/11/2013 → 25/08/2017
Number of participants: 7
Phd Student:
Loureiro da Costa Lira Gargalo, Carina (Intern)
Supervisor:
Carvalho, Ana Isabel C. de Sousa G. (Ekstern)
Gernaey, Krist V. (Intern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
Flores Alsina, Xavier (Intern)
Bezzo, Fabrizio (Ekstern)
Matos, Henrique Aníbal Santos de (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)

Relations
Publications:
Process design, supply chain, economic and environmental analysis for chemical production in a glycerol biorefinery:
Towards the sustainable design of biorefineries
Project: PhD

Biomass gasification in circulating fluidized beds

Department of Chemical and Biochemical Engineering
Period: 01/11/2013 → 31/07/2017
Number of participants: 6
Phd Student:
Seerup, Rasmus (Intern)
Supervisor:
Lin, Weigang (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Larsen, Morten Boberg (Intern)
Song, Wenli (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Linking strain morphology to rheology and mass transfer as a means to improve fermentation processes

Department of Chemical and Biochemical Engineering
Period: 01/11/2013 → 17/05/2017
Number of participants: 8
Phd Student:
Quintanilla Hernandez, Daniela Alejandra (Intern)
Supervisor:
Hansen, Kim (Ekstern)
Hassager, Ole (Intern)
Eliasson Lantz, Anna (Intern)
Development of 2nd Generation Biorefineries Production of Dicarboxylic Acids and Bio-based Polymers Derived Thereof

The existing 2nd generation biorefineries utilize less than 20% of the biomass feedstock for ethanol production, and major side-streams are produced such as pentose and lignin waste streams, that are respectively used for biogas and energy production.

Converting the carbon from these waste streams into added-value products would increase the otherwise low profitability and improve the environmental benefits of the biorefineries. The suggested project BioREFINE-2G aims at developing commercially attractive processes for efficient conversion of pentose-rich side-streams from biorefineries into dicarboxylic acids, which can be used as precursors for bio-based polymers including biodegradable polymers. The project covers the whole value chain, from characterization of side streams from forest and other non-food feedstock, development of novel robust industrial yeast cell factories, fermentation and downstream process development, to polymerization methods development for the production of biodegradable polymers applicable as plastics, coatings or adhesives, scale-up and demonstration and to life cycle and economic viability analyses.

Novo Nordisk Foundation Center for Biosustainability

Applied Metabolic Engineering

Yeast Metabolic Engineering

Quantitative Sustainability Assessment

Department of Management Engineering

Department of Chemical and Biochemical Engineering

CAPEC-PROCESS

Period: 01/10/2013 → 30/09/2017

Number of participants: 7

Acronym: BioREFINE-2G

Project participant:

Stovicek, Vratislav (Intern)

Rasmussen, Birte Kastrup (Intern)

Lis, Alicia Viktoria (Intern)

Lohmann, Ricarda (Intern)

Phd Student:

Ögmundarson, Ólafur (Intern)

Project Coordinator:

Förster, Jochen (Intern)

Borodina, Irina (Intern)

Financing sources

Source: EU research programme (public)

Name of research programme: EU FP7 KBBE

Relations

Activities:

Strain Development for Diacid Production

Publications:

BIOREFINE-2G — Result In Brief: Novel biopolymers from biorefinery waste-streams
CRISPR–Cas system enables fast and simple genome editing of industrial Saccharomyces cerevisiae strains

Project

Migration of bisphenol A from polycarbonate plastic (PC) of different qualities

The survey was decided by the Danish EPA with the aim to study the potential correlation between quality and chemical composition of PC on release of BPA from the material. The study was performed at the Technical University of Denmark in cooperation between DTU National Food Institute and DTU Danish Polymer Centre, Department of Chemical and Biochemical Engineering.

National Food Institute

Division of Risk Assessment and Nutrition

Department of Chemical and Biochemical Engineering

The Danish Polymer Centre

Environmental Protection Agency

Period: 01/10/2013 → 01/05/2015

Number of participants: 3

Project participant:

Petersen, Jens Højslev (Intern)

Hvilsted, Søren (Intern)

Project Manager, academic:

Pedersen, Gitte Alsing (Intern)

Project

Experimental Implementation and model-based optimization for multi-enzyme processes

Department of Chemical and Biochemical Engineering

Period: 01/10/2013 → 15/03/2017

Number of participants: 6

Phd Student:

Abu, Rohana (Intern)

Supervisor:

Gernaey, Krist V. (Intern)

Main Supervisor:

Woodley, John (Intern)

Examiner:

Nordblad, Mathias (Intern)

Blazevic, Zvjezdana Findrik (Ekstern)

Riva, Sergio (Ekstern)

Financing sources

Source: Internal funding (public)

Name of research programme: Stipendie fra udlandet

Relations

Publications:

Process Evaluation Tools for Enzymatic Cascades Welcome Message

Project: PhD

Modeling and Synthesis of Pharmaceutical processes: Moving from Batch to Continuous Manufacturing

Department of Chemical and Biochemical Engineering

Period: 01/10/2013 → 16/11/2016

Number of participants: 7

Phd Student:

Papadakis, Emmanouil (Intern)

Supervisor:

Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Eden, Mario Richard (Intern)
Jiménez-González, Concepción (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Modelling and synthesis of pharmaceutical processes: moving from batch to continuous
Project: PhD

Plantwide modelling and control for N2O emissions from WWTP
Department of Chemical and Biochemical Engineering
Period: 01/10/2013 → 14/12/2016
Number of participants: 6
PhD Student:
Boiocchi, Riccardo (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
Abildskov, Jens (Ekstern)
Weijers, Stefan R. (Ekstern)
van Loosdrecht, Mark (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Publications:
Plant-wide modelling and control of nitrous oxide emissions from wastewater treatment plants
Project: PhD

Supramolecular Polymeric Rheology
Department of Chemical and Biochemical Engineering
Period: 01/10/2013 → 14/12/2016
Number of participants: 6
PhD Student:
Shabbir, Aamir (Intern)
Supervisor:
Skov, Anne Ladegaard (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Creton, Costantino (Ekstern)
Ianniruberto, Giovanni (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Experimental evaluation of carbonic anhydrase as a biocatalyst for implementation in CO2 removal from flue gas

Department of Chemical and Biochemical Engineering
Period: 15/09/2013 → 24/01/2018
Number of participants: 6
PhD Student:
Deslauriers, Maria Gundersen (Intern)
Supervisor:
von Solms, Nicolas (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Pinelo, Manuel (Intern)
Liese, Andreas (Ekstern)
Wentzel, Alexander (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Microcapsules as delivery vehicles

Department of Chemical and Biochemical Engineering
Period: 15/09/2013 → 15/03/2017
Number of participants: 6
PhD Student:
Mazurek, Malgorzata Natalia (Intern)
Supervisor:
Hvilsted, Søren (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Hietala, Sami Heikki Olavi (Ekstern)
Paulsen, Andreas Lundtang (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Pretreatment of hemp fibers for utilization in strong biocomposite materials

Department of Chemical and Biochemical Engineering
Period: 15/09/2013 → 25/01/2017
Number of participants: 6
PhD Student:
Liu, Ming (Intern)
Supervisor:
Thygesen, Anders (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Østergård, Hanne (Intern)
Hotchkiss, Jr., Arland Tillotson (Ekstern)
Tovborg, Morten (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet

**Relations**
Publications:
Pretreatment of hemp fibers for utilization in strong biocomposite materials
Project: PhD

**Automatic design of primers for miR-specific RT-qPCR**
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 02/09/2013 → …
Number of participants: 1
Acronym: miRprimer
Project participant:
Busk, Peter Kamp (Intern)

**Design, control and analysis of intensified biochemical processes**
Department of Chemical and Biochemical Engineering
Period: 01/09/2013 → 16/11/2016
Number of participants: 7
PhD Student:
Mansouri, Seyed Soheil (Intern)
Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
von Solms, Nicolas (Intern)
Lee, Jay Hyung (Ekstern)
Ricardez-Sandoval, Luis (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

**Relations**
Publications:
Integrated Process Design, Control and Analysis of Intensified Chemical Processes
Project: PhD

**Low Temperature Thermal Gasification of High-Alkali Bio Residues and Sludge**
Department of Chemical and Biochemical Engineering
Period: 01/09/2013 → 26/04/2017
Number of participants: 8
Phd Student:
Thomsen, Tobias Pape (Intern)
Supervisor:
Hauggaard-Nielsen, Henrik (Intern)
Henriksen, Ulrik Birk (Intern)
Holm, Jens Kai (Intern)
Main Supervisor:
Ahrenfeldt, Jesper (Intern)
Examiner:
Astrup, Thomas Fruegaard (Intern)
Hindsgaul, Claus (Intern)
Skoglund, Nils (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

Relations
Publications:
Closing the Loop - Utilization of Secondary Resources by Low Temperature Thermal Gasification
Project: PhD

Generic model-based tailor-made design and analysis of biphasic reacting systems
Department of Chemical and Biochemical Engineering
Period: 01/08/2013 → 24/10/2016
Number of participants: 6
Phd Student:
Anantpinijwatna, Amata (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Huusom, Jakob Kjøbsted (Intern)
Grosjean, Christophe (Ekstern)
Manenti, Flavio (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet

Relations
Publications:
Generic Model-Based Tailor-Made Design and Analysis of Biphasic Reaction Systems
Project: PhD

Modeling and Operation of Diesel Engine Exhaust Gas Cleaning Systems
Department of Chemical and Biochemical Engineering
Period: 01/08/2013 → 17/05/2017
Number of participants: 7
Phd Student:
Åberg, Andreas (Intern)
Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Widd, Anders G. (Ekstern)
Main Supervisor:
Abildskov, Jens (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

Relations
Publications:
Modelling and Operation of Diesel Engine Exhaust Gas Cleaning Systems
Project: PhD

New Catalytic materials for combined particulate and NOx removal

Department of Chemical and Biochemical Engineering
Period: 01/07/2013 → 30/04/2018
Number of participants: 5
Phd Student:
Linde, Kasper (Intern)
Supervisor:
Gabrielsson, Pär (Ekstern)
Hansen, Brian Brun (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

An experimental and theoretical study of CO2 hydrate formation systems

Department of Chemical and Biochemical Engineering
Period: 01/06/2013 → 21/06/2017
Number of participants: 6
Phd Student:
Tzirakis, Fragkiskos (Intern)
Supervisor:
von Solms, Nicolas (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Thomsen, Kaj (Intern)
Herri, Jean-Michel (Ekstern)
Lindeloff, Niels (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

Relations
Publications:
An Experimental and Theoretical Study of CO2 Hydrate Formation Systems
Project: PhD

Property Modelling and Process Design involving complex chemical systems

Department of Chemical and Biochemical Engineering
Property Model-based Tailor-made Design of Chemical-based Products
Project: PhD

Synthesis and design of Water/watertower networks
Department of Chemical and Biochemical Engineering
Period: 01/05/2013 → 31/12/2017
Number of participants: 6
Phd Student:
Handani, Zainatul Bahiyah (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Woodley, John (Intern)
Georgiadis, Michael C. (Ekstern)
Mujtaba, Iqbal M. (Ekstern)

Finance sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Development of New Diesel Oxidation and NH3 Slip Catalysts
Department of Chemical and Biochemical Engineering
Period: 01/04/2013 → 30/09/2017
Number of participants: 6
Phd Student:
Hansen, Thomas Klint (Intern)
Supervisor:
Hansen, Brian Brun (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Abildskov, Jens (Ekstern)
Christensen, Kurt Agerbæk (Ekstern)
Skoglundh, Bo Magnus (Ekstern)

Finance sources
**Relations**

Publications:

Development of New Diesel Oxidation and NH$_3$ Slip Catalysts

Project: PhD

**Extensional Rheology of Model Polymers**

Department of Chemical and Biochemical Engineering

Period: 01/04/2013 → 16/06/2016

Number of participants: 7

Phd Student:

Hengeller, Ludovica (Intern)

Supervisor:

Almdal, Kristoffer (Intern)

Skov, Anne Ladegaard (Intern)

Main Supervisor:

Hassager, Ole (Intern)

Examiner:

Szabo, Peter (Intern)

Ianniruberto, Giovanni (Ekstern)

Vlassopoulos, Dimitrios (Intern)

**Financing sources**

Source: Internal funding (public)

Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

**Relations**

Publications:

Entangled Polymer Melts in Extensional Flow

Project: PhD

**Characterization and production of protein isolates from oil-cold-pressed hemp seed meal**

Department of Chemical and Biochemical Engineering

Center for BioProcess Engineering

Period: 25/02/2013 → 12/07/2013

Number of participants: 1

Hemp protein isolates

Main Supervisor:

Ale, Marcel Tutor (Intern)

Project

**Mixing and oxygen transfer processes in bioreactors**

Department of Chemical and Biochemical Engineering

Period: 15/01/2013 → 30/06/2016

Number of participants: 6

Phd Student:

Nørregaard, Anders (Intern)

Supervisor:

van den Berg, Frans W.J. (Intern)

Madsen, Brian (Ekstern)

Stocks, Stuart M. (Ekstern)

Woodley, John (Intern)

Main Supervisor:

Gernaey, Krist V. (Intern)
Synthesis and Evaluation of Structures Lipids based Polyurethanes for Sensors, Actuators and Generators trough Monte Carlo Simulation

Department of Chemical and Biochemical Engineering
Period: 15/01/2013 → 26/05/2016
Number of participants: 7
Phd Student:
Zakaria, Shamsul Bin (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Gernaey, Krist V. (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Jager, Edwin Willem Harm (Ekstern)
Sarban, Rahimullah (Intern)

Mechanically invisible encapsulations

Department of Chemical and Biochemical Engineering
Period: 15/12/2012 → 14/03/2016
Number of participants: 6
Phd Student:
Mazurek, Piotr Stanislaw (Intern)
Production of Prebiotic oligosaccharides by novel enzymatic catalysis
Department of Chemical and Biochemical Engineering
Period: 15/12/2012 → 26/05/2016
Number of participants: 6
Phd Student:
Nordvang, Rune Thorbjørn (Intern)
Supervisor:
Jers, Carsten (Intern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Lange, Lene (Intern)
Bornscheuer, Uwe (Ekstern)
Derkx, Patrick M.F. (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Mechanically invisible encapsulations
Project: PhD

Exploring biochemical process performance limits through topology optimization
Department of Chemical and Biochemical Engineering
Period: 01/12/2012 → 16/06/2016
Number of participants: 7
Phd Student:
Larsson, Hilde Kristina (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Skov, Anne Ladegaard (Intern)
Main Supervisor:
Krühne, Ulrich (Intern)
Examiner:
Sin, Gürkan (Intern)
Drønen, Nils Kjetil (Intern)
Nopens, Ingmar (Ekstern)

Financial sources
Relations
Publications:
Modelling of Mass Transfer Phenomena in Chemical and Biochemical Reactor Systems using Computational Fluid Dynamics
Project: PhD

Gas-Solid reactions and reactor systems
Department of Chemical and Biochemical Engineering
Period: 01/12/2012 → 26/05/2016
Number of participants: 7
PhD Student:
Azizaddini, Seyednezamaddin (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Lin, Weigang (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Henriksen, Ulrik Birk (Intern)
Li, Songgeng (Ekstern)
Erik Weinell, Claus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet

Relations
Publications:
A New Type of Non-Mechanical Valves for Recirculation of Fine Particles
Project: PhD

Generic interface development and benchmarking of carbon dioxide reduction processes
Department of Chemical and Biochemical Engineering
Period: 01/12/2012 → 20/09/2016
Number of participants: 8
PhD Student:
Gaspar, Jozsef (Intern)
Supervisor:
Jørgensen, John Bagterp (Intern)
Thomsen, Kaj (Intern)
von Solms, Nicolas (Intern)
Main Supervisor:
Fosbøl, Philip Loldrup (Intern)
Examiner:
Skiadas, Ioannis V (Intern)
Douglas, Peter (Ekstern)
Gabrielsen, Jostein (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

Relations
Publications:
CO₂ Capture Dynamic and Steady-State Model Development, Optimization and Control: Applied to Piperazine and Enzyme Promoted MEA/MDEA
**High Temperature Process for Energy Conversion**

Department of Chemical and Biochemical Engineering  
Period: 01/12/2012 → 30/04/2017  
Number of participants: 3  
Phd Student: Nordby, Mads Willemoes (Intern)  
Supervisor: Lin, Weigang (Intern)  
Main Supervisor: Dam-Johansen, Kim (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet  
Project: PhD

**Combined soil carbon sequestration and crop nutrient supply using thermal conversion technology residuals**

Department of Chemical and Biochemical Engineering  
Period: 15/11/2012 → 31/12/2014  
Number of participants: 3  
Phd Student: Hansen, Veronika (Intern)  
Supervisor: Ahrenfeldt, Jesper (Intern)  
Main Supervisor: Hauggaard-Nielsen, Henrik (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU) Samf.  
Project: PhD

**Carbohydrate degradation products within biorefining**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2012 → 30/09/2016  
Number of participants: 7  
Phd Student: Rasmussen, Helena (Intern)  
Supervisor: Egsgaard, Helge (Intern)  
Sørensen, Hanne Risbjerg (Ekstern)  
Main Supervisor: Meyer, Anne S. (Intern)  
Examiner: Gavala, Hariklia N. (Intern)  
Taarning, Esben (Intern)  
Willför, Stefan Mikael (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Ansat eksternt  

**Relations**

Publications:  
Carbohydrate degradation mechanisms and compounds from pretreated biomass  
Project: PhD
Reactive Separation Technology: Biometric Enzyme Immobilization

Department of Chemical and Biochemical Engineering
Period: 01/11/2012 → 02/05/2016
Number of participants: 6
PhD Student:
Marpani, Fauziah Binti (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Main Supervisor:
Koutsouris, Georgios (Intern)
Examiner:
Christensen, Jakob Munkholt (Intern)
Jönsson, Ann-Sofi (Extern)
Pedersen, Lars Hastrup (Extern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra uilandet
Project: PhD

Topology optimization in biocatalytic reactions using miniaturized reactors

Department of Chemical and Biochemical Engineering
Period: 01/11/2012 → 20/04/2016
Number of participants: 7
PhD Student:
Pereira Rosinha Grundtvig, Ines (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Woodley, John (Intern)
Main Supervisor:
Krühne, Ulrich (Intern)
Examiner:
Abildskov, Jens (Extern)
Maier, Petra (Extern)
Perozziello, Gerardo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Enzymatic polishing and modification of lignin

Department of Chemical and Biochemical Engineering
Period: 01/10/2012 → 05/01/2018
Number of participants: 6
PhD Student:
Munk, Line (Intern)
Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Kepp, Kasper Planeta (Intern)
Barsberg, Søren (Extern)
Polikarpov, Igor (Extern)
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Mastering bioprocess Integration and Intensification across scales
Department of Chemical and Biochemical Engineering
Period: 01/10/2012 → 02/12/2015
Number of participants: 7
Phd Student:
Ringborg, Rolf Hoffmeyer (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Krühne, Ulrich (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Nordblad, Mathias (Intern)
Hessel, Volker (Ekstern)
Jensen, Klavs F. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Novel clay/nanocellulose biocomposite films and coatings in the context of packaging applications
Department of Chemical and Biochemical Engineering
Period: 01/10/2012 → 20/09/2016
Number of participants: 7
Phd Student:
Trifol Guzman, Jon (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Hassager, Ole (Intern)
Main Supervisor:
Szabo, Peter (Intern)
Examiner:
Skov, Anne Ladegaard (Intern)
Niska, A. Kristiina Oksman (Ekstern)
Rojas, Orlando (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)

Relations
Publications:
Hybrid nanocellulose/nanoclay composites for food packaging applications
Project: PhD

Simultaneous fast pyrolysis and in situ hydrogenation of lignin to obtain a marine diesel fuel
Department of Chemical and Biochemical Engineering
Period: 01/10/2012 → 14/03/2016
Number of participants: 7
Phd Student:
Zhou, Guofeng (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Knudsen, Niels Ole (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Hansen, Brian Brun (Intern)
Seshan, Kulathuiyer (Ekstern)
Taarning, Esben (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

**Enhancing micronutrient bioavailability via designed in situ enzyme catalysis**

Department of Chemical and Biochemical Engineering
Period: 15/09/2012 → 02/12/2015
Number of participants: 5
Phd Student:
Nielsen, Anne Veller Friis (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Lange, Lene (Intern)
Hotchkiss, Jr., Arland Tillotson (Ekstern)
Skov, Lars Kobberøe (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

**Logistics for Energy Crops’ Biomass**

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 01/09/2012 → 31/12/2015
Number of participants: 1
Acronym: LogistEC
Project participant:
Østergård, Hanne (Intern)

**Modeling of Salt Solubility/dissolution in waterflooding of Petroleum Reservoirs**

Department of Chemical and Biochemical Engineering
Period: 01/09/2012 → 18/08/2016
Number of participants: 6
Phd Student:
Chakravarty, Krishna Hara (Intern)
Supervisor:
Fosbøl, Philip Loldrup (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
von Solms, Nicolas (Intern)
Tuxen, Anders (Ekstern)
Zahid, Adeel (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

**Relations**
Publications:

**Modelling of Salt Solubilities for Smart Water flooding in Carbonate Reservoirs using Extended UNIQUAC Model**
Project: PhD

**Modelling of Salinity Effects on Waterflooding of Petroleum Reservoirs**
Department of Chemical and Biochemical Engineering
Period: 01/09/2012 → 26/05/2016
Number of participants: 6
Phd Student:
Alexeev, Artem (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Nielsen, Sidsel Marie (Intern)
Berenblyum, Roman (Ekstern)
Mackay, Erik James (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

**Relations**
Publications:

**Modeling of Salinity Effects on Waterflooding of Petroleum Reservoirs**
Project: PhD

**Model of Stickiness in Spray Drying**
Department of Chemical and Biochemical Engineering
Period: 01/09/2012 → 27/01/2016
Number of participants: 7
Phd Student:
Petersen, Thomas (Intern)
Supervisor:
Sloth, Jakob (Intern)
Ullom, Thorvald Uhrskov (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Szabo, Peter (Intern)
Roos, Yrijö Henrik (Ekstern)
Schuck, Pierre (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU

**Relations**
Publications:

**Model Stickiness in Spray Drying**
Project: PhD
Operation and Design of Diabatic distillation Processes

Department of Chemical and Biochemical Engineering
Period: 01/09/2012 → 16/06/2016
Number of participants: 7
PhD Student:
Bisgaard, Thomas (Intern)
Supervisor:
Pilegaard, Kim (Intern)
von Solms, Nicolas (Intern)
Main Supervisor:
Abildskov, Jens (Ekstern)
Examiner:
Rodriguez-Donis, Ivonne (Intern)
Kiss, Anton Alexandru (Ekstern)
Lee, Jay Hyung (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Process intensification in biocatalytic reactions

Department of Chemical and Biochemical Engineering
Period: 01/09/2012 → 22/02/2016
Number of participants: 7
PhD Student:
Heintz, Søren (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Woodley, John (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Abildskov, Jens (Ekstern)
Straathof, Adrie J.J. (Ekstern)
Wohlgemuth, Roland (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Valorization of Lignin from Biorefineries for Fuels and Chemicals

Department of Chemical and Biochemical Engineering
Period: 01/09/2012 → 25/01/2017
Number of participants: 8
PhD Student:
Nielsen, Joachim Bachmann (Intern)
Supervisor:
Nielsen, John (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Hansen, Brian Brun (Intern)
Nielsen, John (Intern)
Taarning, Esben (Intern)
A soft and conductive PDMS-PEG block copolymer as a compliant electrode for the dielectric elastomer

Soft conducting elastomers have been prepared from polydimethylsiloxane-polyethyleneglycol (PDMS-PEG) copolymer and surfactant-stabilized multi-walled carbon nanotubes (MWCNTs). The copolymer was chain-extended with PDMS of molecular weight 17.2 kg mol⁻¹ in order to obtain a crosslinkable PDMS with molecular weight around 20 – 30 kg mol⁻¹. MWCNTs were treated with surfactant and sonicated for better dispersion in the polymer matrix. The conductivity and mechanical properties of conducting elastomers were thoroughly investigated including stress and strain at break. The developed conducting elastomers showed high conductivity combined with inherent softness. The high conductivity and softness, PDMS- PEG copolymers with incorporated MWCNTs hold great promises as compliant and highly stretchable electrodes for stretchable devices such as electro-mechanical transducers.

Department of Chemical and Biochemical Engineering

Monolithic structures and their influence on electromechanical breakdown phenomena

Department of Chemical and Biochemical Engineering

Synthesis and development of novel coating components for exterior wood applications based on sustainable resources

Department of Chemical and Biochemical Engineering
Period: 01/08/2012 → 22/02/2016
Number of participants: 6

Phd Student:
Nguyen, Hiep Dinh (Intern)

Supervisor:
Hvilsted, Søren (Intern)

Main Supervisor:
Daugaard, Anders Egede (Intern)

Examiner:
Skov, Anne Ladegaard (Intern)
Johansson, Mats (Ekstern)
Paulsen, Andreas Lundtang (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet

Relations
Publications:
Bio-based alkyds by direct enzymatic bulk polymerization
Project: PhD

The MacroAlgaeBiorefinery 3G (MAB3) - sustainable production of 3G bioenergy carriers and high value aquatic fish feed from macroalgae

Department of Chemical and Biochemical Engineering
Period: 15/06/2012 → 18/08/2016
Number of participants: 6

Phd Student:
Manns, Dirk Martin (Intern)

Supervisor:
Saake, Bodo (Ekstern)

Main Supervisor:
Meyer, Anne S. (Intern)

Examiner:
Lange, Lene (Intern)
Horn, Svein Jarle (Ekstern)
SLET - Kádár, Zsófia (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Sourcing and bioprocessing of brown seaweed for maximizing glucose release
Project: PhD

Extraction of protein and amino acid from hemp seed meal

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 01/06/2012 → 30/06/2014
Number of participants: 3

Project participant:
Ale, Marcel Tutor (Intern)
Meyer, Anne S. (Intern)
Pinelo, Manuel (Intern)

Financing sources
Source: Other public support (public)
Name of research programme: **GUDP projects**

**Project**

**Thermodynamic modeling of CO2 hydrates**

Department of Chemical and Biochemical Engineering  
Period: 01/06/2012 → 26/05/2016  
Number of participants: **5**  
Phd Student:  
Bjørner, Martin Gamel (Intern)  
Main Supervisor:  
Kontogeorgis, Georgios (Intern)  
Examiner:  
von Solms, Nicolas (Intern)  
Gross, Joachim (Ekstern)  
Karakatsani, Eirini (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering

**Relations**

Publications:  
Thermodynamic modeling of CO2 mixtures  

Project: PhD

**Integrated framework for synthesis and design of multi-product biorefinery networks**

Department of Chemical and Biochemical Engineering  
Period: 01/05/2012 → 01/07/2015  
Number of participants: **6**  
Phd Student:  
Cheali, Peam (Intern)  
Supervisor:  
Gernaey, Krist V. (Intern)  
Main Supervisor:  
Sin, Gürkan (Intern)  
Examiner:  
Huusom, Jakob Kjøbsted (Intern)  
Mogensen, Johan (Ekstern)  
Zondervan, Edwin (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU) Samf.  
Project: PhD

**Modelling and Simulation of Wastewater Treatment Plants**

Department of Chemical and Biochemical Engineering  
Period: 01/05/2012 → 01/07/2015  
Number of participants: **9**  
Phd Student:  
Snip, Laura (Intern)  
Supervisor:  
Alsina, Xavier Flores (Ekstern)  
Jeppsson, Ulf A. C. (Ekstern)  
Krühne, Ulrich (Intern)  
Plósz, Benedek G. (Intern)  
Main Supervisor:
Wood Coatings

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering

CERE – Center for Energy Resources Engineering
Period: 01/05/2012 → 30/11/2016
Number of participants: 1
Project ID: 50902
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

Single Biomass Particle Combustion and Fuel Characterization

Department of Chemical and Biochemical Engineering
Period: 01/04/2012 → 18/08/2016
Number of participants: 8
Phd Student:
Trubetskaya, Anna (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Jensen, Anker Degn (Intern)
Shapiro, Alexander (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Ahrenfeldt, Jesper (Intern)
Thunman, Henrik (Ekstern)
Wadenbäck, Johan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Fast pyrolysis of biomass at high temperatures
Project: PhD

Systematic Methods and Tools for Computer Aided Modeling

Department of Chemical and Biochemical Engineering
Period: 01/04/2012 → 02/09/2015
Number of participants: 6
Phd Student:
Fedorova, Marina (Intern)
Supervisor:
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Examiner:
Gernaey, Krist V. (Intern)
Linninger, Andreas A. (Ekstern)
Preisig, Heinz A. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

In-Optics Humidity Compensation of NDIR Measurements for Combustion Emission Gas Sensing and Analysis

Department of Chemical and Biochemical Engineering
Period: 15/02/2012 → 16/12/2015
Number of participants: 7
Phd Student:
Stolberg-Rohr, Thomine Kirstine (Intern)
Supervisor:
Glarborg, Peter (Intern)
Skov Hansen, René (Intern)
Main Supervisor:
Clausen, Sønnik (Intern)
Examiner:
Lindvold, Lars René (Intern)
Fabricius, Henrik (Ekstern)
Li, Zhongshan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU

Relations
Publications:
NOx Monitoring in Humid Exhaust Gas Using Non-Dispersive Infrared Spectroscopy
Project: PhD

CHIGP Petrobras
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Period: 01/02/2012 → 31/12/2014
Number of participants: 2
Project ID: 50894
Other:
Biede, Anne Louise (Intern)
Project Manager, organisational:
Kontogeorgis, Georgios (Intern)

Application of waste streams with high ash content in the cement industry

Department of Chemical and Biochemical Engineering
Period: 01/02/2012 → 30/04/2013
Number of participants: 4
Phd Student:
Bagh, David (Intern)
Bioprocess engineering for the application of P450s
Department of Chemical and Biochemical Engineering
Period: 01/02/2012 → 02/12/2015
Number of participants: 6
PhD Student:
Lundemo, Marie Therese (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Eliasson Lantz, Anna (Intern)
Hayes, Martin (Ekstern)
Schmid, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

CHIGP Petrobras
Funded by Petrobras
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/02/2012 → 31/12/2014
Number of participants: 1
Project ID: 50894
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

CO2 Kompression
Funded by Lloyds Register
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/02/2012 → 31/12/2012
Number of participants: 1
Project ID: 50893
Project Manager, academic:
Fosbøl, Philip Loldrup (Intern)
Development of Non Destructive Methods
Funded by "Fonden for ikke-destruktiv prøvning"

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Period: 01/02/2012 → 31/03/2016
Number of participants: 1
Project Manager, academic:
Fosbøl, Philip Loldrup (Intern)

Enchanced Oil Recovery with Application of Microorganisms
Department of Chemical and Biochemical Engineering
Period: 01/02/2012 → 01/07/2015
Number of participants: 7
Phd Student:
Halim, Amalia Yunita (Intern)
Supervisor:
Eliasson Lantz, Anna (Intern)
Nielsen, Sidse Marie (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Yan, Wei (Intern)
Alkan, Hakan (Ekstern)
Zahid, Adeel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Modelling of phase equilibria and related properties of mixtures involving lipids
Department of Chemical and Biochemical Engineering
Period: 01/02/2012 → 13/05/2015
Number of participants: 6
Phd Student:
Cunico, Larissa (Intern)
Supervisor:
Sarup, Bent (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Sales Cruz, Alfonso Mauricio (Intern)
Jaubert, Jean-Noel (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Computer aided framework for synthesis, design and retrofit of water networks in processing industries
Department of Chemical and Biochemical Engineering
Period: 16/12/2011 → 13/05/2015
Number of participants: 6
Phd Student:
Bozkurt, Hande (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
Krühne, Ulrich (Intern)
Comas, Joaquim (Ekstern)
Weijers, Stefan R. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Novel Small Scale Biogas Concepts for Local Waste handling and Energy Production in Greenland
Department of Chemical and Biochemical Engineering
Period: 15/12/2011 → 31/10/2013
Number of participants: 5
Phd Student:
Heiske, Stefan (Intern)
Supervisor:
Jensen, Pernille Erland (Intern)
Kiørboe, Lars Georg (Intern)
Kroff, Pablo (Intern)
Main Supervisor:
Østergård, Hanne (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

selective and efficient synthesis of ethanol from dimethyl ether and syngas
Department of Chemical and Biochemical Engineering
Period: 15/12/2011 → 30/09/2015
Number of participants: 11
Phd Student:
Rasmussen, Dominik Bjørn (Intern)
Supervisor:
Christensen, Jakob Munkholt (Intern)
Moses, Poul Georg (Intern)
Riisager, Anders (Intern)
Rossmeisl, Jan (Intern)
Studt, Felix (Intern)
Temel, Burcin (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Jensen, Peter Arendt (Intern)
Sehested, Jens (Intern)
Swang, Ole (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD
Hot-Embossing on silicon elastomers
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Period: 01/12/2011 → …
Number of participants: 1
Project participant:
Vudayagiri, Sindhu (Intern)

Enhanced Oil Recovery with Application of Enzymes
Department of Chemical and Biochemical Engineering
Period: 01/12/2011 → 26/05/2016
Number of participants: 6
Phd Student:
Khusainova, Alsu (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Yan, Wei (Intern)
Ivar Andersen, Simon (Intern)
Skauge, Arne (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed

Relations
Publications:
Enhanced Oil Recovery with Application of Enzymes
Project: PhD

Fuel Efficiency and Fouling Control Coatings in Maritime Transport
Department of Chemical and Biochemical Engineering
Period: 01/12/2011 → 30/09/2015
Number of participants: 8
Phd Student:
Lindholdt, Asger (Intern)
Supervisor:
Kiil, Søren (Intern)
Olsen, Stefan Møller (Intern)
Meseguer Yebra, Diego (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Dame, Anne Juul (Intern)
Hoffmann, Markus (Ekstern)
Swain, Geoffrey W. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD
Microalgae withincreased synthesis or diminish breakdown of triacylglycerol for efficient biodiesel production

Department of Chemical and Biochemical Engineering
Period: 01/12/2011 → 30/11/2013
Number of participants: 5
Phd Student:
Favrholdt, Camilla Emilie (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Gjermansen, Claes (Intern)
Woodley, John (Intern)
Main Supervisor:
Brandt, Anders Bøving (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

On-line trace gas measurement technique for gasification

Department of Chemical and Biochemical Engineering
Period: 01/12/2011 → 25/03/2015
Number of participants: 6
Phd Student:
Grosch, Helge (Intern)
Supervisor:
Clausen, Sønnik (Intern)
Main Supervisor:
Fateev, Alexander (Intern)
Examiner:
Dame, Anne Juul (Intern)
Ebert, Volker (Ekstern)
Neubauer, York (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Optimizing the anaerobic digestion of manure

Department of Chemical and Biochemical Engineering
Period: 01/12/2011 → 01/07/2015
Number of participants: 6
Phd Student:
Sun, Guotao (Intern)
Supervisor:
Thygesen, Anders (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Jørgensen, Henning (Intern)
Jensen, Jens Oluf (Intern)
Kroff, Pablo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD
**Thermal conversion technology for biomass and waste and their potential in the Chinese energy market**

Department of Chemical and Biochemical Engineering  
Period: 01/12/2011 → 11/08/2013  
Number of participants: 2  
PhD Student:  
Kallestrup, Kasper Bislev (Intern)  
Main Supervisor:  
Dam-Johansen, Kim (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet  
Project: PhD

**CO2 Hydrates-Challenges and Possibilities**  
While great efforts are undertaken in oil and gas exploration to inhibit the formation of hydrates which may lead to production stops, it has been suggested that in relation to carbon capture, hydrate formation should instead be actively stimulated. A joint CERE/Ecole des Mines (France) project addresses both challenges and possibilities.

Funded by FIST  
Center for Energy Resources Engineering  
Department of Chemical and Biochemical Engineering  
CERE – Center for Energy Resources Engineering  
Period: 08/11/2011 → 30/06/2014  
Number of participants: 1  
Project ID: 50868  
Project Manager, academic:  
Kontogeorgis, Georgios (Intern)

**Lignin derived phenolics**  
Department of Chemical and Biochemical Engineering  
Period: 01/11/2011 → 10/09/2012  
Number of participants: 3  
PhD Student:  
Weiss, Noah Daniel (Intern)  
Supervisor:  
Sørensen, Hanne Risbjerg (Ekstern)  
Main Supervisor:  
Meyer, Anne S. (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Ansat eksternt  
Project: PhD

**Otto Mønsted**  
Funded by Otto Mønsted’s Fond  
Center for Energy Resources Engineering  
Department of Chemical and Biochemical Engineering  
CERE – Center for Energy Resources Engineering  
Period: 01/10/2011 → 31/12/2012  
Number of participants: 1  
Project ID: 50863  
Project Manager, academic:
Process Technology for Oxidase-based Biocatalysis
Department of Chemical and Biochemical Engineering
Period: 01/10/2011 → 26/11/2014
Number of participants: 6
Phd Student:
Ramesh, Hemalata (Intern)
Supervisor:
Krühne, Ulrich (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Huusom, Jakob Kjøbsted (Intern)
Archer, Ian (Ekstern)
Micheletti, Martina (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Alternative Fuels in Cement Production
Department of Chemical and Biochemical Engineering
Period: 01/09/2011 → 17/12/2014
Number of participants: 7
Phd Student:
Cortada Mut, Maria del Mar (Intern)
Supervisor:
Glarborg, Peter (Intern)
Nørskov, Linda Kaare (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Illerup, Jytte Boll (Intern)
Hupa, Mikko (Ekstern)
Schäfer, Stefan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Control of Enzymatic Biodiesel Production
Department of Chemical and Biochemical Engineering
Period: 01/09/2011 → 26/11/2014
Number of participants: 7
Phd Student:
Price, Jason Anthony (Intern)
Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Nordblad, Mathias (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Phenomena based process intensification

Department of Chemical and Biochemical Engineering
Period: 01/09/2011 → 04/02/2015
Number of participants: 6
Phd Student:
Babi, Deenesh Kavi (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Huusom, Jakob Kjøbsted (Intern)
Sundmacher, Kai (Ekstern)
Van Gerven, Tom (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Power plant burners for biodust combustion

Department of Chemical and Biochemical Engineering
Period: 01/09/2011 → 20/04/2016
Number of participants: 6
Phd Student:
Johansen, Joakim Myung (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Obernberger, Ingwald (Ekstern)
Henriksen, Ulrik Birk (Intern)
Norman, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Wind Turbine Blade Coatings with Anti-Erosion Properties

Department of Chemical and Biochemical Engineering
Period: 01/09/2011 → 26/11/2014
Number of participants: 7
Phd Student:
Zhang, Shizhong (Intern)
Development of new materials for dielectric electroactive polymers as actuators and generators

Department of Chemical and Biochemical Engineering
Period: 15/08/2011 → 26/11/2014
Number of participants: 7
Phd Student:
Madsen, Frederikke Bahrt (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Examiner:
Kiil, Søren (Intern)
Brook, Michael Adrian (Ekstern)
Graz, Ingrid Maria (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Sustainability assessment of 2nd generation bioenergy production in Ghana

Department of Chemical and Biochemical Engineering
Period: 15/08/2011 → 18/08/2016
Number of participants: 5
Phd Student:
Kamp, Andreas (Intern)
Main Supervisor:
Østergård, Hanne (Intern)
Examiner:
Pilegaard, Kim (Intern)
Hauggaard-Nielsen, Henrik (Intern)
Raugei, Marco (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Relations
Publications:
Environmental Sustainability Assessment of Integrated Food and Bioenergy Production with Case Studies from Ghana
Project: PhD
Thermodynamic modelling in oil-sea water mixtures

Department of Chemical and Biochemical Engineering
Period: 15/08/2011 → 26/11/2014
Number of participants: 7
Phd Student:
Liang, Xiaodong (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Yan, Wei (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
von Solms, Nicolas (Intern)
Lindeloff, Niels (Intern)
Sadowski, Gabriele (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Design of continuous reactor systems for API production

Department of Chemical and Biochemical Engineering
Period: 01/08/2011 → 17/12/2014
Number of participants: 7
Phd Student:
Pedersen, Michael Jønch (Intern)
Supervisor:
Kiil, Søren (Intern)
Skovby, Tommy (Ekstern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Kappe, Oliver (Ekstern)
Petersen, Hans (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Development of stimuli-responsive polymer network

Department of Chemical and Biochemical Engineering
Period: 01/08/2011 → 17/12/2014
Number of participants: 6
Phd Student:
Ma, Baoguang (Intern)
Supervisor:
Hvilsted, Søren (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Hietala, Sami Heikki Olavi (Ekstern)
Paulsen, Andreas Lundtang (Intern)

Financing sources
**Inhibition of gas hydrate formation by ice-structuring proteins**

Department of Chemical and Biochemical Engineering  
**Period:** 01/08/2011 → 10/11/2015  
**Number of participants:** 6  
**PhD Student:**  
Malmos Perfeldt, Christine (Intern)  
**Supervisor:**  
Woodley, John (Intern)  
**Main Supervisor:**  
von Solms, Nicolas (Intern)  
**Examiner:**  
Thomsen, Kaj (Intern)  
Li, Xiaoyun (Ekstern)  
Svartås, Thor Martin (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Eksternt finansieret virksomhed  
**Project:** PhD

**Large Scale Processing of dielectric electro active polymers**

Department of Chemical and Biochemical Engineering  
**Period:** 01/08/2011 → 30/09/2014  
**Number of participants:** 7  
**PhD Student:**  
Vudayagiri, Sindhu (Intern)  
**Supervisor:**  
Daugaard, Anders Egede (Intern)  
Kjærboe, Lars Georg (Intern)  
**Main Supervisor:**  
Skov, Anne Ladegaard (Intern)  
**Examiner:**  
Szabo, Peter (Intern)  
Shea, Herbert R. (Ekstern)  
Sommer-Larsen, Peter (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Offentlig finansiering  
**Project:** PhD

**Mechanical characterization methods for dielectric electroactive polymers**

Department of Chemical and Biochemical Engineering  
**Period:** 01/08/2011 → 26/11/2014  
**Number of participants:** 6  
**PhD Student:**  
Goswami, Kaustav (Intern)  
**Supervisor:**  
Daugaard, Anders Egede (Intern)  
**Main Supervisor:**  
Skov, Anne Ladegaard (Intern)  
**Examiner:**  
von Solms, Nicolas (Intern)
Benslimane, Mohamed Yahia (Ekstern)
Opris, Dorina (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

**Optimizing control of the integrated urban wastewater system**
Department of Chemical and Biochemical Engineering
Period: 01/08/2011 → 10/11/2015
Number of participants: 6
Phd Student:
Mollerup, Ane Loft (Intern)
Supervisor:
Mikkelsen, Peter Steen (Intern)
Main Supervisor:
Sin, Gürkan (Intern)
 Examiner:
Gernaey, Krist V. (Intern)
Olsson, Gustaf (Ekstern)
Weijers, Stefan R. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

**Systematic methodology for design of emulsion based chemical products**
Department of Chemical and Biochemical Engineering
Period: 01/08/2011 → 30/09/2014
Number of participants: 6
Phd Student:
Mattei, Michele (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Kate, Antoon J. B. ten (Ekstern)
Wiebe, Lars (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

**Ash Chemistry in Circulating Fluidized Bed**
Department of Chemical and Biochemical Engineering
Period: 01/07/2011 → 24/06/2016
Number of participants: 7
Phd Student:
Narayan, Vikas (Intern)
Supervisor:
Henriksen, Ulrik Birk (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Illerup, Jytte Boll (Intern)
Gøbel, Benny (Intern)
Wang, Liang (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

Relations
Publications:
Ash behavior and de-fluidization in low temperature circulating fluidized bed biomass gasifier
Project: PhD

Deactivation of SCR catalysts in biomass fired power plants
Department of Chemical and Biochemical Engineering
Period: 15/06/2011 → 01/07/2015
Number of participants: 6
PhD Student:
Olsen, Brian Kjærgaard (Intern)
Supervisor:
Castellino, Francesco (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Fehrmann, Rasmus (Intern)
Christensen, Kurt Agerbæk (Ekstern)
Engvall, Klas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Measurement and modelling of phase equilibrium of oil-water,polar chemicals
Department of Chemical and Biochemical Engineering
Period: 01/06/2011 → 11/03/2015
Number of participants: 7
PhD Student:
Frost, Michael Grynnerup (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
von Solms, Nicolas (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Yan, Wei (Intern)
Hendriks, Eric Maria (Ekstern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD
Functional Electrospun Nanostructures and Microstructures for Food and Bioengineering Applications

The objectives of this project is to generate the scientific and technological basis to: (i) develop new nano-microcarrier systems for bioactive compounds using electrospun nano-microstructures for their immobilization, (ii) develop new nano-micronodelivery systems utilizing enzyme functionality and molecular imprinted polymers for controlled delivery/release of bioactives, (iii) study the structural and functional properties of nano-microstructures (NMS) as novel components of food and bioengineered products, (iv) evaluate their bioavailability and degradation/digestion in-vitro and in-vivo.

The overall aim is to create new functional systems that have a potential usage in foods/healthy foods, as nutritional supplements, as pharmaceutical products and for a range of other bioengineering applications. The project’s ambition is also to contribute to research training in research institutes and industrial companies as well as education of industrial employees. We expect that the obtained knowledge will strengthen the Danish industry’s potential to emerging nano-microtechnologies and technologies of bioactives.

National Food Institute
Division of Industrial Food Research
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Period: 01/05/2011 → 31/10/2015
Number of participants: 10
Acronym: FENAMI
Project participant:
Meyer, Anne S. (Intern)
Qvortrup, Klaus (Ekstern)
Ye, Lei (Ekstern)
Goycoolea, F.M. (Ekstern)
Nielsen, Kent Albin (Ekstern)
Jessen, Flemming (Intern)
Boutrup Stephansen, Karen (Intern)
Jørgensen, Lars (Intern)
Mendes, Ana Carina Loureiro (Intern)
Project Manager, academic:
Chronakis, Ioannis S. (Intern)

Financing sources
Source: Public research council
Name of research programme: Danish Research Council/Programme Commission for "Sundhed, Fødevarer og Velfærd"
Amount: 14,866,637.00 Danish Kroner

Relations
Activities:
FENAMI Project Course : Advances in Bioinspired Nanomaterials and Approaches in Life Sciences

Combustion Characterization of Bio-derived Fuels and Additives
Department of Chemical and Biochemical Engineering
Period: 01/05/2011 → 13/05/2015
Number of participants: 6
Phd Student:
Hashemi, Hamid (Intern)
Supervisor:
Christensen, Jakob Munkholt (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Hansen, Brian Brun (Intern)
Alzueta, Maria (Intern)
Kristensen, Per Graves (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

**Mathematical Modelling of vegetable oil crystallisation**

Department of Chemical and Biochemical Engineering  
Period: 01/05/2011 → 27/08/2014  
Number of participants: 7  
Phd Student:  
Hjorth, Jeppe Lindegaard (Intern)  
Supervisor:  
Dam-Johansen, Kim (Intern)  
Leth-Miller, Rasmus (Intern)  
Main Supervisor:  
Kiil, Søren (Intern)  
Examiner:  
Abildskov, Jens (Ekstern)  
Flöter, Eckhard (Ekstern)  
Schafer, Olivier (Ekstern)  

**Financing sources**  
Source: Internal funding (public)

Name of research programme: ErhvervsPhD-ordningen VTU  
Project: PhD

**Symbiotic growth depressions in bioenergy and forage crops**

Department of Chemical and Biochemical Engineering  
Period: 01/04/2011 → 31/12/2014  
Number of participants: 4  
Phd Student:  
Clausen, Signe Sandbech (Intern)  
Supervisor:  
Grønlund, Mette (Intern)  
Lenk, Ingo (Intern)  
Main Supervisor:  
Jakobsen, Iver (Intern)  

**Financing sources**  
Source: Internal funding (public)

Name of research programme: Institut stipendie (DTU) Samf.  
Project: PhD

**Novel greener and lean processes using integrated microfactories**

This project is focusing on efficient and sustainable production of organic-synthesis based active pharmaceutical ingredients (API) by use of novel microfluidic based concepts to biocatalytic and fermentation processes. Major challenges are met since many of these processes have complex reaction mechanisms with equilibrium limited conversions, often substrate and/or product inhibition and material transport challenges along with slow heterogenic reaction kinetics. In this project it is hypothesized that much faster process development could be achieved by studying bioprocesses in continuous flow mode already from the laboratory stage. Well characterized (fast mixing and heat transmission) small reactors with low dead volumes will facilitate dynamic experiments, while non-invasive, real-time, in-line monitoring technologies will provide high quality data, with potential for automation, real-time optimization and rapid modeling of reaction kinetics.

Department of Chemical and Biochemical Engineering  
Center for Process Engineering and Technology  
Period: 01/03/2011 → 28/02/2014  
Number of participants: 3  
biocatalysis, in situ product removal, CFD, microfluidics, kinetic investigations  
Acronym: µ factories  
Number of related Ph.D. students: 1
The water content of natural gas often poses problems during production, transmission and distribution. Use of production chemicals like glycols and alcohols add to complexity. CERE is the academic partner of a collaborative R&D project on the subject initiated by The European Gas Research Group (GERG).

**Integrated microfactories for enzyme production**

Department of Chemical and Biochemical Engineering

Period: 01/03/2011 → 11/03/2015

Number of participants: 7

Phd Student:

Bodla, Vijaya Krishna (Intern)

Supervisor:

Krühne, Ulrich (Intern)

Woodley, John (Intern)

Main Supervisor:

Gernaey, Krist V. (Intern)

Examiner:

Nordblad, Mathias (Intern)

Baganz, Frank (Ekstern)

Bouwes, Dominique (Ekstern)

**Financing sources**

Source: Internal funding (public)

Name of research programme: Forskningsrådsfinansiering

Project: PhD

**Multi-dimensional population balance models of crystallization processes**

Department of Chemical and Biochemical Engineering

Period: 01/03/2011 → 04/02/2015

Number of participants: 7

Phd Student:

Meisler, Kresten Troelstrup (Intern)

Supervisor:

Gernaey, Krist V. (Intern)

von Solms, Nicolas (Intern)

Main Supervisor:

Gani, Rafiqul (Intern)

Examiner:

Krühne, Ulrich (Intern)
Mazzotti, Marco (Ekstern)
Seidel-Morgenstern, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Reson
Funded by Højteknologifonden
DOC 11/03305
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/03/2011 → 31/12/2014
Number of participants: 1
Project ID: 50826
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

Diversity screening for novel enzymes degrading synthetic polymers
Department of Chemical and Biochemical Engineering
Period: 01/02/2011 → 26/11/2014
Number of participants: 7
Phd Student:
Lezyk, Mateusz Jakub (Intern)
Supervisor:
Badia, Antoni Sánchez (Ekstern)
Kiil, Søren (Intern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Eliasson Lantz, Anna (Intern)
Derkx, Patrick M.F. (Ekstern)
Visser, Jacob (Jaap) (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Ph.D. Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects
Funded by: Deltagerbetaling
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/02/2011 → 30/11/2011
Number of participants: 1
Acronym: Ph.D. Kursus MLM
Project Manager, academic:
Kontogeorgis, Georgios (Intern)
**Climate Change Effects to Plant Ecosystems**
Department of Chemical and Biochemical Engineering  
Period: 01/01/2011 → 24/09/2014  
Number of participants: 6  
Phd Student:  
Ingvordsen, Cathrine Heinz (Intern)  
Supervisor:  
Mikkelsen, Teis Nørgaard (Intern)  
Main Supervisor:  
Bagger Jørgensen, Rikke (Intern)  
Examiner:  
Pilegaard, Kim (Intern)  
Ainsworth, Lisa (Ekstern)  
Flavell, Andrew John (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut, samfinansiering  
Project: PhD

**Design and testing of robust and efficient fire-retardant coatings**
Department of Chemical and Biochemical Engineering  
Period: 01/01/2011 → 28/05/2014  
Number of participants: 6  
Phd Student:  
Nørgaard, Kristian Petersen (Intern)  
Supervisor:  
Dam-Johansen, Kim (Intern)  
Main Supervisor:  
Kil, Søren (Intern)  
Examiner:  
Jappe Frandsen, Flemming (Intern)  
Deters, David C. (Ekstern)  
Giovanni, Camino (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet  
Project: PhD

**Development of the next generation biocatalysts for industrial production of chemicals (Bionexgen)**
Department of Chemical and Biochemical Engineering  
Period: 01/01/2011 → 01/01/2013  
Number of participants: 1  
Project Manager, organisational:  
Törnvall, Ulrika (Intern)  

**2nd Generation Bioenergy Production from Waste Resources in Ghana**
Department of Chemical and Biochemical Engineering  
Period: 01/12/2010 → 23/04/2014  
Number of participants: 7  
Phd Student:  
Thomsen, Sune Tjalfe (Intern)  
Supervisor:  
Kroff, Pablo (Intern)  
SLET - Kádár, Zsófia (Ekstern)
Gas Hydrate Inhibition with Ice-Structuring Proteins
Large quantities of gas hydrate inhibitors, primarily methanol and glycol, secure oil recovery under cold and high-pressure conditions. The present CERE project follows up on previous research which suggested that proteins found in bark beetle, meal worm and Arctic fish species might be able to do the job more efficiently.

Funded by FIST
DOC 10/01685

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering

CERE – Center for Energy Resources Engineering
Period: 01/12/2010 → 30/05/2014
Number of participants: 1
Project ID: 50805
Project Manager, academic:
von Solms, Nicolas (Intern)

Project

Large scale enzymatic production of bioactive fibers from potato pulp

Department of Chemical and Biochemical Engineering
Period: 01/12/2010 → 17/12/2014
Number of participants: 7
PhD Student:
Ravn, Helle Christine (Intern)
Supervisor:
Kiørboe, Lars Georg (Intern)
Sørensen, Ole Bandsholm (Ekstern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Mikkelsen, Jørn Dalgaard (Intern)
Hotchkiss, Jr., Arland Tillotson (Ekstern)
Nielsen, Per Munk (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Reactor and Process Design for Multi-enzymatic Synthesis

Department of Chemical and Biochemical Engineering
Period: 01/12/2010 → 01/11/2016
Number of participants: 4
PhD Student:
Xue, Rui (Intern)
Supervisor:
Scale-up of biocatalytic cascade reactions for the synthesis of chiral amines

Department of Chemical and Biochemical Engineering
Period: 01/12/2010 → 24/09/2014
Number of participants: 7
Phd Student:
Janes, Kresimir (Intern)
Supervisor:
Tufvesson, Pär (Intern)
Woodley, John (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Krühne, Ulrich (Intern)
Pedersen, Lars Haastrup (Ekstern)
Vasic-Racki, Durda (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Udbrænding af affald på rist

Department of Chemical and Biochemical Engineering
Period: 01/12/2010 → 30/01/2013
Number of participants: 4
Phd Student:
Jørgensen, Jan Hein (Intern)
Supervisor:
Hassing, Henrik (Ekstern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Operational aspects of continuous pharmaceuical production

Department of Chemical and Biochemical Engineering
Period: 15/11/2010 → 02/07/2014
Number of participants: 7
Phd Student:
Mitic, Aleksandar (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Skovby, Tommy (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Jensen, Anker Degn (Intern)
Aelterman, Wim (Ekstern)
Hessel, Volker (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

A methodology for systematic design and selection of green solvents for increased yield in organic reactions

Department of Chemical and Biochemical Engineering
Period: 01/11/2010 → 31/03/2013
Number of participants: 4
Phd Student:
Mitrofanov, Igor (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Combined silage pretreatment and enzymatic hydrolysis of energy grasses for 2G bioethanol production

Department of Chemical and Biochemical Engineering
Period: 01/11/2010 → 28/05/2014
Number of participants: 7
Phd Student:
Ambye-Jensen, Morten (Intern)
Supervisor:
Didion, Thomas (Ekstern)
Johansen, Katja Salomon (Ekstern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Jørgensen, Henning (Intern)
Galbe, Mats (Ekstern)
Larsen, Jan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Symbolic Communities, Increase of Biomass and Biodiesel Production

Department of Chemical and Biochemical Engineering
Period: 01/11/2010 → 26/11/2014
Number of participants: 6
Phd Student:
Baggesen, Claus (Intern)
Supervisor:
Brandt, Anders Bøving (Intern)
Main Supervisor:
Gjermansen, Claes (Intern)
Examiner:
Pilegaard, Kim (Intern)
Albers, Eva (Ekstern)
Møller, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Udvikling af ny teknik til fosfor-indvinding fra aske fra forbrænding af spildevandsslam
Section for Construction Materials
Department of Civil Engineering
Department of Chemical and Biochemical Engineering
Period: 15/10/2010 → 15/10/2011
Number of participants: 5
Project ID: 26132
Project participant:
Jensen, Pernille Erland (Intern)
Kirkelund, Gunvor Marie (Intern)
Christensen, Iben Vernegren (Intern)
Dama, Anne Juul (Intern)
Project Manager, organisational:
Ottosen, Lisbeth M. (Intern)

Financing sources
Source: Forskningsprojekter - Miljø- og Energiministeriet
Name of research programme: Forskningsprojekter - Miljø- og Energiministeriet
Amount: 390,000.00 Danish Kroner
Project

Thermodynamic Modeling for CO2 Capture Systems
Department of Chemical and Biochemical Engineering
Number of participants: 6
Phd Student:
Arshad, Muhammad Waseem (Intern)
Supervisor:
von Solms, Nicolas (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Karlsson, Hans T. (Ekstern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Nitrogen cycle assessments and greenhouse gas emission in low-input legume managements
Department of Chemical and Biochemical Engineering
Period: 01/09/2010 → 11/12/2013
Number of participants: 6


**Validation of Structures Model for Autotrophic Nitrogen Removal in High Strength Wastewater**

Department of Chemical and Biochemical Engineering

Period: 01/09/2010 → 12/11/2013

Number of participants: 7

Phd Student:

Vangsgaard, Anna Katrine (Intern)

Supervisor:

Gernaey, Krist V. (Intern)

Main Supervisor:

Sin, Gürkan (Intern)

Examiner:

Krühne, Ulrich (Intern)

Lemaire, Romain (Ekstern)

Morgenroth, Eberhard (Ekstern)

**Financing sources**

Source: Internal funding (public)

Name of research programme: Anden EU-finansiering

Project: PhD

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**Catalytic Conversion of Bio-oil to Fuel for Transportation**

Department of Chemical and Biochemical Engineering

Period: 15/08/2010 → 23/04/2014

Number of participants: 7

Phd Student:

Mortensen, Peter Mølgaard (Intern)

Supervisor:

Grunwaldt, Jan-Dierk (Intern)

Jensen, Peter Arendt (Intern)

Main Supervisor:

Jensen, Anker Degn (Intern)

Examiner:

Riisager, Anders (Intern)

Gabrielsen, Jostein (Intern)

Murzin, Dmitry (Ekstern)

**Financing sources**

Source: Internal funding (public)

Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

Project: PhD
Catalytic Steam reforming of Bio-Oil to Hydrogen Rich Gas

Department of Chemical and Biochemical Engineering
Period: 15/08/2010 → 18/12/2013
Number of participants: 6
Phd Student:
Trane-Restrup, Rasmus (Intern)
Supervisor:
Dahl, Søren (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Jensen, Peter Arendt (Intern)
Grunwaldt, Jan-Dierk (Intern)
Østberg, Martin (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Enzymatic Production of Human Milk Oligosaccharides

Department of Chemical and Biochemical Engineering
Period: 15/08/2010 → 24/09/2014
Number of participants: 6
Phd Student:
Guo, Yao (Intern)
Supervisor:
Willer, Martin (Intern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Pinelo, Manuel (Intern)
Rasmussen, Søren Kjærgård (Intern)
Schols, Henk (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Substrate-based selection of enzymes

Department of Chemical and Biochemical Engineering
Period: 15/08/2010 → 23/04/2014
Number of participants: 6
Phd Student:
Dominiak, Malgorzata Maria (Intern)
Supervisor:
Sworm, Graham (Ekstern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Pinelo, Manuel (Intern)
Schols, Henk (Ekstern)
Ulvskov, Peter (Ekstern)

Financing sources
Climate Change Mitigation by Plant mediated transfer and storage of carbon in aquifers

Department of Chemical and Biochemical Engineering
Period: 01/08/2010 → 11/12/2013
Number of participants: 6
Phd Student:
Thaysen, Eike Marie (Intern)
Supervisor:
Ambus, Per (Intern)
Main Supervisor:
Jakobsen, Iver (Intern)
Examiner:
Ibrom, Andreas (Intern)
Bertrand, Isabelle (Ekstern)
Manning, David Andrew Charles (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of an Electrolyte CPA Equation of state for Applications in the Petroleum and Chemical Industries

Department of Chemical and Biochemical Engineering
Period: 01/08/2010 → 02/07/2014
Number of participants: 6
Phd Student:
Maribo-Mogensen, Bjørn (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
von Solms, Nicolas (Intern)
Anderko, Andrzej (Ekstern)
Hemptinne, Jean-Charles de (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

PhD Project in Membrane Technology

Department of Chemical and Biochemical Engineering
Period: 01/08/2010 → 31/01/2012
Number of participants: 3
Phd Student:
Kulkarni, Anant (Ekstern)
Supervisor:
Pinelo, Manuel (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Tailor-made design of chemical products: Bio-fuels and other blended products

Department of Chemical and Biochemical Engineering
Period: 15/07/2010 → 07/05/2014
Number of participants: 7
PhD Student:
Yunus, Nor Alafiza Binti (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Sin, Gürkan (Intern)
Harper, Peter Mathias (Intern)
Kate, Antoon J. B. ten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlantet

Model Based Integrated Process-Product Design - retrofitting and optimisation

Department of Chemical and Biochemical Engineering
Period: 01/07/2010 → 30/09/2013
Number of participants: 8
PhD Student:
Hukkerikar, Amol Shivajirao (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Gani, Rafiqul (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Frenkel, Michael (Ekstern)
Krooshof, Gerard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt

Analysis and Quantification of Foaming Phenomena in Wet Flue Gas Desulphurization Plants

Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 03/02/2014
Number of participants: 6
PhD Student:
Qin, Siqiang (Intern)
Supervisor:
Hansen, Brian Brun (Intern)
Main Supervisor:
Kil, Søren (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Incremental refinement of process design
Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 30/09/2013
Number of participants: 7
Phd Student:
Quaglia, Alberto (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
Jørgensen, John Bagterp (Intern)
Bode, Andreas (Ekstern)
Pistikopoulos, Efstratios N. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Novel Analytical Technologies
Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 30/09/2013
Number of participants: 6
Phd Student:
Baum, Andreas (Intern)
Supervisor:
Hansen, Per Waaben (Ekstern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Berg, Marco A. Van den (Ekstern)
van den Berg, Frans W.J. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt EU-finansieret

Relations
Publications:
Descriptive and predictive assessment of enzyme activity and enzyme related processes in biorefinery using IR spectroscopy and chemometrics
Project: PhD

Physiological responses of plants and ecosystems to climate change
Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 30/09/2013
Number of participants: 6
Phd Student:
Boesgaard, Kristine Stove (Intern)
Supervisor:
Ibrom, Andreas (Intern)
Ro-Poulsen, Helge (Ekstern)
Examiner:
Pilegaard, Kim (Intern)
Calfapietra, Carlo (Ekstern)
Ottosen, Carl-Otto (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Process Considerations for Asymmetric Synthesis of Chiral Amines using Omega-Transaminase

Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 11/12/2013
Number of participants: 6
Phd Student:
Lima Afonso Neto, Watson (Intern)
Supervisor:
Tufvesson, Pär (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Krühne, Ulrich (Intern)
Adlercreutz, Patrick (Ekstern)
Howard, Roger M. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Thermodynamic Modelling of Regenerative Fuel Cell Energy Storage Systems

Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 30/09/2012
Number of participants: 2
Phd Student:
Cuthbert, Sean Vernon (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

**CLEO Forskningsprojekt**
Funded by TNO
DOC 08/03100

Under lukning

Center for Energy Resources Engineering
BioSOFC - 3rd Generation Biomass Based Combined Heat and Power (CHP)
The aim of project is to investigate the combination of biomass gasification with SOFC in an efficient decentralized and flexible energy system for small scale combined heat and power production. The project work includes design, construction and long term operation of a gasifier-SOFC stack test set-up, analysis of performance and system analysis.

Department of Mechanical Engineering
Energy Engineering
Rise National Laboratory for Sustainable Energy
Department of Chemical and Biochemical Engineering
Biosystems Division
CHEC Research Centre
Biomass Gasification
Department of Energy Conversion and Storage
Fuel Cells and Solid State Chemistry Division
Applied Electrochemistry
Electrochemical Evaluation

Strategies for Organic and Low-input Integrated Breeding and Management
DTU role: WP leader of WP8: Environmental, economic and social sustainability assessment leader, Member of WP1:, WP2:, WP4:

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

SOLIBAM

Project
Guiding biocatalytic process improvements using engineering evaluation tools

Department of Chemical and Biochemical Engineering
Period: 01/03/2010 → 24/06/2013
Number of participants: 6
Phd Student:
Lima Ramos, Joana (Intern)
Supervisor:
Tufvesson, Pär (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Jiménez-González, Concepción (Ekstern)
Straathof, Adrie J.J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Monitoring Continuous fermentation processes in microbioreactors

Department of Chemical and Biochemical Engineering
Period: 01/03/2010 → 14/03/2018
Number of participants: 8
Phd Student:
Bolic, Andrijana (Intern)
Supervisor:
Eliasson Lantz, Anna (Intern)
Rottwitt, Karsten (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Dufva, Martin (Intern)
Dufva, Martin (Intern)
Roca, Christophe Francois Aime (Intern)
Roca, Christophe Francois Aime (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

New Polymer Architectures for Proton Conducting Fuel Cell Membranes

Department of Chemical and Biochemical Engineering
Period: 01/03/2010 → 21/05/2013
Number of participants: 6
Phd Student:
Nielsen, Mads Møller (Intern)
Supervisor:
Jankova Atanasova, Katja (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Skov, Anne Ladegaard (Intern)
Jones, Deborah (Ekstern)
Tenhu, Heikki Juhani (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Substrate-based selection of enzymes
Department of Chemical and Biochemical Engineering
Period: 01/03/2010 → 22/10/2014
Number of participants: 5
Phd Student:
Feng, Tao (Intern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Hobley, Timothy John (Intern)
Berg, Marco A. van den (Ekstern)
Pedersen, Lars Hastrup (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Molecular Rheology of Complex Fluids
Department of Chemical and Biochemical Engineering
Period: 01/02/2010 → 19/04/2013
Number of participants: 7
Phd Student:
Huang, Qian (Intern)
Supervisor:
Rasmussen, Henrik K. (Intern)
Skov, Anne Ladegaard (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Ianniruberto, Giovanni (Ekstern)
Vlassopoulos, Dimitrios (Intern)

Financial sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Thermodynamic and Process Modelling of Gas Hydrate Systems in CO2 Capture Processes
Department of Chemical and Biochemical Engineering
Period: 01/02/2010 → 26/02/2014
Number of participants: 7
Phd Student:
Herslund, Peter Jørgensen (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Thomsen, Kaj (Intern)
Main Supervisor:
von Solms, Nicolas (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Hendriks, Eric Maria (Ekstern)
Peter, Englezos (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Catalytic Synthesis of Alcoholic Fuels for Transportation from Syngas
Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 19/03/2013
Number of participants: 7
Phd Student:
Wu, Qiongxiao (Intern)
Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Temel, Burcin (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Riisager, Anders (Intern)
Hinrichsen, Kai-Olaf (Ekstern)
Østberg, Martin (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

CHIGP DONG
Funded by DONG Energy
DOC 10/00681
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Period: 01/01/2010 → 31/03/2013
Number of participants: 1
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

Innovative CO2 Capture
Funded by NTNU/EU 7
DOC 10/01054
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Period: 01/01/2010 → 30/06/2014
Number of participants: 1
Acronym: EU ICAP
Project ID: 50751
Project Manager, academic:
von Solms, Nicolas (Intern)

Relations
Publications:
Freezing Point Depressions of Phase Change CO2 Solvents
Heat of Absorption of CO2 in Phase Change Solvents: 2-(Diethylamino)ethanol and 3-(Methylamino)propylamine

Measurements and Modeling of Thermodynamics of Organic Sulfur Species in Hydrocarbons and Pure Water
Funded by FIST
DOC 09/01183

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/01/2010 → 31/12/2012
Number of participants: 1
Acronym: CHIGP Sulfur
Project ID: 50707
Project Manager, academic:
Awan, Javeed (Intern)

Model for deposition build-up in biomass boilers
Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 22/02/2016
Number of participants: 7
Phd Student:
Hansen, Stine Broholm (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Dane, Anne Juul (Intern)
Gupta, Rajender (Ekstern)
Jensen, Jørgen Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet

Relations
Publications:
Model for Deposition Build-up in Biomass Boilers
Project: PhD

Pre-heater design in cement plant for high energy efficiency and low emissions
Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 26/02/2014
Number of participants: 7
Phd Student:
Maarup, Claus (Intern)
Supervisor:
Clement, Karsten (Intern)
Hjuler, Klaus (Ekstern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Kiørboe, Lars Georg (Intern)
Hustad, Johan Einar (Ekstern)
Stoltze, Sten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Processes for Low CO2 Emissions
Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 18/12/2013
Number of participants: 8
Phd Student:
Pathi, Sharat Kumar (Intern)
Supervisor:
Hjuler, Klaus (Ekstern)
Illerup, Jytte Boll (Intern)
Lin, Weigang (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Kiil, Søren (Intern)
Jensen, Lars Skaarup (Intern)
Murillo, Ramón (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Production, Refining and Utilization of Biomass for Energy Services
Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 26/02/2014
Number of participants: 7
Phd Student:
Saleh, Suriyati Binti (Intern)
Supervisor:
Hansen, Brian Brun (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Ahrenfeldt, Jesper (Intern)
Brink, Anders Stig (Ekstern)
Holm, Jens Kai (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Separation of Chiral Active Pharmaceutical Ingredients: A First Step Towards Continuous Preferential Crystallization in the Pharmaceutical Industry
Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 24/06/2013
Number of participants: 7
Phd Student:
Systemic approach to sustainability assessment of food and bioenergy production in a societal context

Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 30/09/2013
Number of participants: 5
PhD Student:
Markussen, Mads Ville (Intern)
Main Supervisor:
Østergård, Hanne (Intern)
Examiner:
Pilegaard, Kim (Intern)
Bastianoni, Simone (Ekstern)
Rasmussen, Kjeld (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Treatment of Lignin and Waste Residues by Flash Pyrolysis

Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 30/09/2013
Number of participants: 6
PhD Student:
Trinh, Ngoc Trung (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Jensen, Lars Skaarup (Intern)
Spliethoff, Hartmut (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Upgrading Fuel Properties of Biomass Fuel and Waste by Torrefaction

Department of Chemical and Biochemical Engineering
Heterogeneously catalysed reactions in supercritical carbon dioxide as innovative and greensolvent

SILP enzyme catalysis technology for upgrading of biomass C5 monomers
**Long Term Climate Change Effects on Dynamics of Microorganisms and Carbon in the Root Zone**

Department of Chemical and Biochemical Engineering  
Period: 01/12/2009 → 19/03/2013  
Number of participants: 6  
PhD Student:  
Reinsch, Sabine (Intern)  
Supervisor:  
Jakobsen, Iver (Intern)  
Main Supervisor:  
Ambus, Per (Intern)  
Examiner:  
Pilegaard, Kim (Intern)  
Olsson, Pål Axel (Ekstern)  
Zechmeister-Boltenstern, Sophie (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet  
Project: PhD

**Ecological modelling: Effects of Climatic Variability and extreme events on carbon cycling in terristrial ecosystem**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2009 → 01/03/2013  
Number of participants: 7  
PhD Student:  
Wu, Jian (Intern)  
Supervisor:  
Beier, Claus (Intern)  
vander Linden, Leon (Intern)  
Main Supervisor:  
Ibrom, Andreas (Intern)  
Examiner:  
Ambus, Per (Intern)  
Bøgh, Eva (Ekstern)  
Smith, Benjamin (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut, samfinansiering  
Project: PhD

**Modelling controled release of substrate and removal of products in biocatalysis**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2009 → 21/05/2013  
Number of participants: 7  
PhD Student:  
Al-Haque, Naweed (Intern)  
Supervisor:  
Gani, Rafiqul (Intern)  
Tufvesson, Pär (Intern)  
Main Supervisor:  
Woodley, John (Intern)  
Examiner:  
Krühne, Ulrich (Intern)
Daugulis, Andrew J. (Ekstern)
Spiess, Antje C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Population balance models and computational fluid dynamics: a model framework to describe heterogeneity in fermentors

Department of Chemical and Biochemical Engineering
Period: 01/11/2009 → 19/03/2013
Number of participants: 7
Phd Student:
Lencastre Fernandes, Rita (Intern)
Supervisor:
Jensen, Anker Degn (Intern)
Nopens, Ingmar (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Ekstern)
Examiner:
Woodley, John (Intern)
Hansen, Ernst (Intern)
Kremling, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Stochastic Modelling Polydisperse Transport of Particles in Porous Media

Department of Chemical and Biochemical Engineering
Period: 01/10/2009 → 17/12/2012
Number of participants: 6
Phd Student:
Yuan, Hao (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Szabo, Peter (Ekstern)
Bradford, Scott Alan (Ekstern)
Lindeloff, Niels (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Complex Phase Behavior and Modeling of Multicomponent Mixtures Containing CO2
Funded by Gassco
DOC 09/02510

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/09/2009 → 01/06/2012
Number of participants: 1
Nanoparticle synthesis using flame spray pyrolysis for catalysis

Department of Chemical and Biochemical Engineering
Period: 01/09/2009 → 28/01/2013
Number of participants: 7
Phd Student:
Høj, Martin (Intern)
Supervisor:
Elmøe, Tobias Dokkedal (Intern)
Grunwaldt, Jan-Dierk (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Fehrmann, Rasmus (Intern)
Christensen, Kurt Agerbæk (Ekstern)
Schomäcker, Reinhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

ParPor - Particles in Pores. Stochastic Modeling of Polydisperse Transport
Particle transport in porous media takes place in a range of contexts, i.e. industrial filtration, waste water treatment, mass transfer in human tissues, mud filtration around oil wells and others. Based on a stochastic approach the CERE project develops software for practical use in modeling of flows of suspensions in porous media.

Funded by FIST
DOC 09/01186

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/09/2009 → 31/08/2012
Number of participants: 1
Acronym: ParPor
Project ID: 50711
Project Manager, academic:
Shapiro, Alexander (Intern)

Process development: Enzymatic upgrading of pectin from sugar beet pulp

Department of Chemical and Biochemical Engineering
Period: 01/06/2009 → 04/09/2013
Number of participants: 6
Phd Student:
Ahmadi Gavlighi, Hassan (Intern)
Supervisor:
Meyer, Anne S. (Intern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Chronakis, Ioannis S. (Intern)
Stimuli-Adaptable Materials

Department of Chemical and Biochemical Engineering
Period: 01/05/2009 → 21/05/2013
Number of participants: 7
PhD Student:
Frankær, Sarah Maria Grundahl (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Kiil, Søren (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Examiner:
Hvilsted, Søren (Intern)
Hansen, Kristoffer Karsten (Intern)
Hietala, Sami (Ekstern)

Development and Analysis of Group-Constribustion plus Models for Property Prediction of Organic Chemical Systems

Department of Chemical and Biochemical Engineering
Period: 01/04/2009 → 19/03/2013
Number of participants: 6
PhD Student:
Mustaffa, Azizul Azri (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Abildskov, Jens (Ekstern)
Voutsas, Epaminondas C. (Ekstern)
Wiebe, Lars (Ekstern)

Optical Tomography in Combustion

Department of Chemical and Biochemical Engineering
Period: 01/04/2009 → 21/05/2013
Number of participants: 6
PhD Student:
Evseev, Vadim (Intern)
Supervisor:
Fateev, Alexander (Intern)
Main Supervisor:
Clausen, Sønnik (Intern)
Examiner:
Glarborg, Peter (Intern)
Hult, Johan Fredrik (Ekstern)
Li, Zhongshan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

**Thermodynamic Modelling of Acid Gases - Alkanolamine Systems**

Department of Chemical and Biochemical Engineering
Period: 01/04/2009 → 21/05/2013
Number of participants: 6
Phd Student:
Sadegh, Negar (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Knudsen, Kim (Intern)
Koch, Oliver (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**Undersøgelse af effekten af alternative enzymproduktionsteknologier**

Department of Chemical and Biochemical Engineering
Period: 01/04/2009 → 27/06/2012
Number of participants: 7
Phd Student:
Albæk, Mads Orla (Intern)
Supervisor:
Hansen, Morten Skov (Intern)
Stocks, Stuart M. (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Ekstern)
Examiner:
Villadsen, John (Intern)
Grøn, Susanne (Intern)
Lübbert, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

**Evaluation of new process technology for lipase-catalyzed biodiesel production**

Department of Chemical and Biochemical Engineering
Period: 01/03/2009 → 27/06/2012
Number of participants: 6
Phd Student:
Xu, Yuan (Intern)  
Supervisor:  
Nordblad, Mathias (Intern)  
Main Supervisor:  
Woodley, John (Intern)  
Examiner:  
Hobley, Timothy John (Intern)  
Basheer, Sobhi (Ekstern)  
Hua, Ling (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Offentlig finansiering  
Project: PhD

**Discovery, Characterization and Design of a thermostable RGI Lyase for production of Bio-Functional Fibers**  
Department of Chemical and Biochemical Engineering  
Period: 01/02/2009 → 18/12/2013  
Number of participants: 6  
Phd Student:  
da Silva, Ines Isabel Cardoso Rodrigues (Intern)  
Supervisor:  
Meyer, Anne S. (Intern)  
Main Supervisor:  
Mikkelsen, Jørn Dalgaard (Intern)  
Examiner:  
Pinelo, Manuel (Intern)  
Kragh, Karsten M. (Ekstern)  
Visser, Jacob (Jaap) (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Globaliseringsmidler  
Project: PhD

**Advanced Waterflooding in Low Permeable Carbonate Reservoirs**  
Department of Chemical and Biochemical Engineering  
Period: 01/01/2009 → 27/06/2012  
Number of participants: 7  
Phd Student:  
Zahid, Adeel (Intern)  
Supervisor:  
Stenby, Erling Halfdan (Intern)  
Yan, Wei (Intern)  
Main Supervisor:  
Shapiro, Alexander (Intern)  
Examiner:  
Thomsen, Kaj (Intern)  
Christensen, Helle Foged (Intern)  
Spildo, Kristine (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Eksternt finansieret virksomhed  
Project: PhD

**Biomass and Coal Gasification in entrained-flow reactor**
Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 01/03/2013
Number of participants: 7
Phd Student:
Qin, Ke (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Lin, Weigang (Intern)
Main Supervisor:
Jensen, Anker Degin (Intern)
Examiner:
Henriksen, Ulrik Birk (Intern)
Engvall, Klas (Ekstern)
Jensen, Jørgen Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Brændselstilfældige brænder til cement- og mineralindustri

Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 17/12/2012
Number of participants: 8
Phd Student:
Nørskov, Linda Kaare (Intern)
Supervisor:
Giarborg, Peter (Intern)
Jensen, Peter Arendt (Intern)
Larsen, Morten Boberg (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Brink, Anders Stig (Ekstern)
Emberger, Bernhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Control of Process Operations and Monitoring of Product Qualities through Hybrid Multi-Scale Model-Based Analysis

Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 21/11/2012
Number of participants: 7
Phd Student:
Abdul Samad, Noor Asma Fazli Bin (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, John Bagterp (Intern)
Georgiadis, Michael C. (Ekstern)
Kalman Nagy, Zoltan (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

PhD Summer School
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/01/2009 → 31/12/2015
Number of participants: 1
Project ID: 50671
Project Manager, academic:
Shapiro, Alexander (Intern)
Project

Polymer Dynamics in Microfluidic Devices
Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 18/04/2012
Number of participants: 7
Phd Student:
Hansen, Rasmus (Intern)
Supervisor:
Bruus, Henrik (Intern)
Callisen, Thomas Hønger (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Anna, Shelley Lynn (Ekstern)
Olmsted, Peter D. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Reactive Transport in Oil Recovery Processes
Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 31/05/2011
Number of participants: 4
Phd Student:
Jain, Priyanka (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
von Solms, Nicolas (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Self-Healing anticorrosive coatings
Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 20/08/2012
Number of participants: 7
Phd Student:
Nesterova, Tatyana (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Pedersen, Lars Thorslund (Intern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Rasmussen, Søren Nyborg (Ekstern)
Zwaag, Sybrand van der (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Smart Waterflooding in Carbonate Reservoirs
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/01/2009 → 28/02/2012
Number of participants: 2
Phd Student:
Zahid, Adeel (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)

Soddannelse i tårkeder
Department of Chemical and Biochemical Engineering
Period: 12/12/2008 → 12/12/2008
Number of participants: 6
Phd Student:
Pedersen, Kim Hougaard (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Main Supervisor:
Jensen, Anker Degrn (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Bech, Nicolai (Ekstern)
Hupa, Mikko (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

CO 2 capture from flue gas using amino acid salt solutions
Department of Chemical and Biochemical Engineering
Period: 01/12/2008 → 21/11/2012
Number of participants: 6
Phd Student:
Lerche, Benedicte Mai (Intern)
Computer-aided modelling for efficient and innovative product-process engineering

Department of Chemical and Biochemical Engineering
Period: 01/12/2008 → 18/04/2012
Number of participants: 7
PhD Student:
Heitzig, Martina (Intern)
Supervisor:
Glarborg, Peter (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Piccione, Patrick M. (Ekstern)
Pistikopoulos, Stratos (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Green Chemistry based innovative process-operation synthesis and design

Department of Chemical and Biochemical Engineering
Period: 01/12/2008 → 18/04/2012
Number of participants: 6
PhD Student:
Lutze, Philip (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Berg, Henk van den (Ekstern)
Freund, Hannsjörg (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Fundamental Understanding of Biomass Pelletization

Department of Chemical and Biochemical Engineering
Multi-enzyme process modelling

Department of Chemical and Biochemical Engineering
Period: 01/11/2008 → 27/06/2012
Number of participants: 7
Phd Student:
Andrade Santacoloma, Paloma de Gracia (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Pedersen, Sven (Ekstern)
Vasic-Racki, Durda (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Prediction of flow induced inhomogeneities in self compacting concrete

The main objective of the project is to improve the basic understanding of the flow behaviour of SCC. The research will produce tools allowing for the prediction of the casting process itself (formwork filling and formwork pressure) along with the prediction of the occurrence of hidden defects such as heterogeneities and weak interfaces. The project will result in a modelling framework for numerical simulation of full scale casting of SCC. The framework will be established through a cross disciplinary collaboration. A project sponsored by the Danish Research Council

Section for Construction Materials
Department of Civil Engineering
Department of Mechanical Engineering
The Danish Polymer Centre
Department of Chemical and Biochemical Engineering
Period: 01/11/2008 → 31/10/2012
Number of participants: 6
Project ID: 25990
Project participant:
Stang, Henrik (Intern)
Roussel, Nicolas (Ekstern)
Production and purification of prebiotic oligosaccharides by chromatography and membrane systems

Department of Chemical and Biochemical Engineering
Period: 01/11/2008 → 28/05/2014
Number of participants: 7
Phd Student:
Michalak, Malwina (Intern)
Supervisor:
Jonsson, Gunnar Eigil (Intern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Examiner:
Jørgensen, Henning (Intern)
Sabesan, Subramaniam (Ekstern)
Wejse, Peter Langborg (Ekstern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 4,179,427.00 Danish Kroner

Production and Utilisation of Hemicelluloses from Renewable Resources for Sustainbale Advanced Products

Department of Chemical and Biochemical Engineering
Period: 15/09/2008 → 18/04/2012
Number of participants: 6
Phd Student:
Sárossy, Zsuzsa (Intern)
Supervisor:
Egsgaard, Helge (Intern)
Main Supervisor:
Plackett, David (Intern)
Examiner:
Ndoni, Sokol (Intern)
Edlund, Ulrica (Ekstern)
Sanadi, Anand R. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Globaliseringsmidler

Characterization and quantification of deposits build up and removal in straw suspension fired boilers

Department of Chemical and Biochemical Engineering
Period: 01/09/2008 → 30/09/2012
Number of participants: 8
Phd Student:
Shafique Bashir, Muhammad (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Jensen, Peter Arendt (Intern)
Wedel, Stig (Ekstern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Glarborg, Peter (Intern)
Jensen, Jørgen Peter (Intern)
Tran, Honghi (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Multiphase flows in porous media
Department of Chemical and Biochemical Engineering
Period: 01/09/2008 → 14/12/2011
Number of participants: 5
Phd Student:
Zhang, Xuan (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Yan, Wei (Intern)
Øbro, Hans (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Optimization of Tailor-made Chemicals from Renewable and non-renewable sources
Department of Chemical and Biochemical Engineering
Period: 01/09/2008 → 01/02/2010
Number of participants: 4
Phd Student:
Swangkotchakorn, Chutima (Intern)
Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Enzymatic Production of Gut-functional Polysaccharides
Department of Chemical and Biochemical Engineering
Period: 01/08/2008 → 27/06/2012
Number of participants: 5
Phd Student:
### Moving from batch towards continuous organic-chemical pharmaceutical production

*Department of Chemical and Biochemical Engineering*

**Period:** 01/08/2008 → 08/02/2012  
**Number of participants:** 8  
**Phd Student:**  
Cervera Padrell, Albert Emili (Intern)  
**Supervisor:**  
Gani, Rafiqul (Intern)  
Kiil, Søren (Intern)  
Skovby, Tommy (Ekstern)  
**Main Supervisor:**  
Gernaey, Krist V. (Intern)  
**Examiner:**  
Jensen, Anker Degn (Intern)  
Aelterman, Wim (Ekstern)  
Hartman, Ryan L. (Ekstern)

**Financing sources**  
*Source:* Internal funding (public)  
*Name of research programme:* Stipendie fra udlandet  
*Project:* PhD

### Systematic Modelling, Simulation and Design of Intensified Bio-Chemical Processes

*Department of Chemical and Biochemical Engineering*

**Period:** 01/08/2008 → 29/11/2011  
**Number of participants:** 6  
**Phd Student:**  
Roman Martinez, Alicia (Intern)  
**Supervisor:**  
Woodley, John (Intern)  
**Main Supervisor:**  
Gani, Rafiqul (Intern)  
**Examiner:**  
Gernaey, Krist V. (Intern)  
Sales Cruz, Alfonso Mauricio (Intern)  
Wiebe, Lars (Ekstern)

**Financing sources**  
*Source:* Internal funding (public)  
*Name of research programme:* Institut stipendie (DTU)  
*Project:* PhD

### Polymer Design and Processing for Liquid Core Waveguides

*Department of Chemical and Biochemical Engineering*
Period: 15/07/2008 → 08/02/2012
Number of participants: 7
Phd Student:
Sagar, Kaushal Shashikant (Intern)
Supervisor:
Christiansen, Mads Brøkner (Intern)
Ndoni, Sokol (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Jankova Atanasova, Katja (Intern)
Geschke, Oliver (Intern)
Grützner, Gabi (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Optimal Waste Slag handling: Minimizing heavy metal leaching and deposit corrosion
Department of Chemical and Biochemical Engineering
Period: 01/06/2008 → 31/12/2008
Number of participants: 3
Phd Student:
Bøjer, Martin (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Computer Modelling of Lipid Processing Technology
Department of Chemical and Biochemical Engineering
Period: 01/05/2008 → 29/11/2011
Number of participants: 6
Phd Student:
Diaz Tovar, Carlos Axel (Intern)
Supervisor:
Sarup, Bent (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Sin, Gürkan (Intern)
Balchen, Steen (Intern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Enhanced Oil Recovery with Surfactant Flooding
Department of Chemical and Biochemical Engineering
Period: 01/05/2008 → 27/06/2012
Number of participants: 6
Phd Student:
Sandersen, Sara Bülow (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
von Solms, Nicolas (Intern)
Examiner:
Yan, Wei (Intern)
Skauge, Arne (Ekstern)
Sparsø, Flemming Vang (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Enzymatic Upgrading of Plant Biomass
Department of Chemical and Biochemical Engineering
Period: 01/05/2008 → 30/09/2013
Number of participants: 6
Phd Student:
Tsai, Chien Tai (Intern)
Supervisor:
Johansen, Katja Salomon (Ekstern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Jensen, Peter Arendt (Intern)
Lidén, Gunnar (Ekstern)
Olsen, Hans Sejr (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Mercury Chemistry in Flue Gas
Department of Chemical and Biochemical Engineering
Period: 01/05/2008 → 18/04/2012
Number of participants: 7
Phd Student:
Madsen, Karin (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Jensen, Joakim Reimer (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Wedel, Stig (Ekstern)
Jensen, Jørgen Peter (Intern)
Senior, Constance L. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD
Valued Added Chemicals from Biomass by Heterogeneous Catalysis

Department of Chemical and Biochemical Engineering
Period: 01/05/2008 → 21/09/2011
Number of participants: 7
Phd Student: Voss, Bodil (Intern)
Supervisor: Grunwaldt, Jan-Dierk (Intern)
Schjødt, Niels Christian (Ekstern)
Main Supervisor: Woodley, John (Intern)
Examiner: Jensen, Anker Degn (Intern)
Jakobsson, Niklas (Ekstern)
Patience, Gregory S. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Distribution of Complex Chemicals in Oil-Water Systems

Department of Chemical and Biochemical Engineering
Period: 01/04/2008 → 08/02/2012
Number of participants: 7
Phd Student: Riaz, Muhammad (Intern)
Supervisor: Stenby, Erling Halfdan (Intern)
Yan, Wei (Intern)
Main Supervisor: Kontogeorgis, Georgios (Intern)
Examiner: von Solms, Nicolas (Intern)
Hemptinne, Jean-Charles de (Ekstern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Enzymatic Production of Dietary Fibres and Prebiotics from Potato Pulp

Department of Chemical and Biochemical Engineering
Period: 01/04/2008 → 24/08/2011
Number of participants: 5
Phd Student: Stouby, Lise (Intern)
Main Supervisor: Meyer, Anne S. (Intern)
Examiner: Adler-Nissen, Jens (Intern)
Hotchkiss, Arland (Ekstern)
Lærke, Helle Nyaagaard (Ekstern)

Financing sources
Mercury removal from cement plant by sorbent injection upstream of pulse jet fabric filter

Department of Chemical and Biochemical Engineering  
Period: 01/04/2008 → 14/12/2011  
Number of participants: 6  
Phd Student:  
Zheng, Yuanjing (Intern)  
Supervisor:  
Windelin, Christian (Ekstern)  
Main Supervisor:  
Jensen, Anker Degn (Intern)  
Examiner:  
Johnsson, Jan Erik (Intern)  
Larsen, Morten Boberg (Intern)  
Strömberg, Dan (Ekstern)

Financing sources
Source: Internal funding (public)  
Name of research programme: ErhvervsPhD-ordningen VTU  
Project: PhD

Rotérovndesign til maksimal brug af alternative brændsler i cement- og mineralindustri

Department of Chemical and Biochemical Engineering  
Period: 01/04/2008 → 08/02/2012  
Number of participants: 7  
Phd Student:  
Nielsen, Anders Rooma (Intern)  
Supervisor:  
Glarborg, Peter (Intern)  
Larsen, Morten Boberg (Intern)  
Main Supervisor:  
Dam-Johansen, Kim (Intern)  
Examiner:  
Clement, Karsten (Intern)  
Leckner, Bo (Ekstern)  
Sander, Bo (Ekstern)

Financing sources
Source: Internal funding (public)  
Name of research programme: ErhvervsPhD-ordningen VTU  
Project: PhD

Membrane Assisted Enzyme Fractionation

Department of Chemical and Biochemical Engineering  
Period: 15/03/2008 → 08/02/2012  
Number of participants: 8  
Phd Student:  
Yuan, Linfeng (Intern)  
Supervisor:  
Jakobsen, Sune (Intern)  
Korsholm, Lars (Ekstern)  
Woodley, John (Intern)  
Main Supervisor:  
Jonsson, Gunnar Eigil (Intern)
Examining:
Gernaey, Krist V. (Intern)
Kristensen, Steen (Ekstern)
Thom, Volkmar (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

**Biofuels from Nuisance Marine Algae**
Department of Chemical and Biochemical Engineering
Period: 01/03/2008 → 18/04/2012
Number of participants: 5
PhD Student:
Ale, Marcel Tutor (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Jacobsen, Charlotte (Ekstern)
Saake, Bodo (Ekstern)
Troelsen, Jesper Thorvald (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

**Clinker Burning Kinetics and Mechanisms**
Department of Chemical and Biochemical Engineering
Period: 01/03/2008 → 24/05/2012
Number of participants: 7
PhD Student:
Telschow, Samira (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Wedel, Stig (Ekstern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Jensen, Peter Arendt (Intern)
Hupa, Mikko (Ekstern)
Jensen, Lars Skaarup (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**Discovery of new thermophilic enzymes for production of dietary fibres and prebiotics from plant material resioves**
Department of Chemical and Biochemical Engineering
Period: 01/03/2008 → 30/09/2014
Number of participants: 5
PhD Student:
Larsen, Dorte Møller (Intern)
Main Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
reactor and process design for chem.-enzymatic synthesis of FDA

Department of Chemical and Biochemical Engineering
Period: 01/03/2008 → 18/04/2012
Number of participants: 6
Phd Student:
Fu, Wenjing (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Lye, Gary J. (Ekstern)
Wiebe, Lars (Ekstern)

Catalytic reactions in Supercritical Fluids

Department of Chemical and Biochemical Engineering
Period: 15/02/2008 → 13/04/2011
Number of participants: 7
Phd Student:
Beier, Matthias Josef (Intern)
Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Riisager, Anders (Intern)
Herbst, Konrad (Ekstern)
Muhler, Martin (Ekstern)

CO2 Capture with Aqueous Ammonia

Department of Chemical and Biochemical Engineering
Period: 01/02/2008 → 14/12/2011
Number of participants: 7
Phd Student:
Darde, Victor Camille Alfred (Intern)
Integrated modelling for simulation and design of novel enzymatic processes

An increasing number of industrially relevant enzymatic processes, including the production of biofuels, prebiotics and new chemicals by "green chemistry", use solid or very viscous plant material as the raw material. These processes all depend on the parallel and/or serial action of multiple enzyme activities to produce the end products. Currently, the development and transfer of these processes from the proof-of-concept bench-scale stage to industrial scale are mainly done empirically and based on experiences from conventional one-pot conversion processes. This approach is rather inefficient and costly in terms of time and resource investments and may not even offer the most optimal and sustainable solutions.

To resolve these challenges, this project aims to introduce a more rational model-based simulation framework for enzyme process design.

Department of Chemical and Biochemical Engineering
Period: 01/02/2008 → 31/07/2010
Number of participants: 1
Project ID: 50551
Project Manager, organisational:
Sin, Gürkan (Intern)

Financing sources
Source: Forskningsprojekter - Andre ministerier og styrelser
Name of research programme: Forskningsprojekter - Andre ministerier og styrelser
Amount: 1,886,400.00 Danish Kroner
Project

Nanoscopic Polymer Membranes

Department of Chemical and Biochemical Engineering
Period: 01/02/2008 → 24/08/2011
Number of participants: 7
Phd Student:
Li, Li (Intern)
Supervisor:
Clausen, Lydia Dahl (Ekstern)
Ndoni, Sokol (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Almdal, Kristoffer (Intern)
Hansen, Thomas (Intern)
Ulbricht, Mathias (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD
Thermodynamic Properties and Phase Equilibria from Fluctuation Solution Theory

Department of Chemical and Biochemical Engineering
Period: 01/02/2008 → 15/06/2011
Number of participants: 5
Phd Student:
Ellegaard, Martin Dela (Intern)
Main Supervisor:
Abildskov, Jens (Ekstern)
Examiner:
Kontogeorgis, Georgios (Intern)
Crafts, Peter (Ekstern)
Sadowski, Gabriele (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Enzymatic Production of Prebiotics from Sugar Beet Pectin

Department of Chemical and Biochemical Engineering
Number of participants: 6
Phd Student:
Holck, Jesper (Intern)
Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Jonsson, Gunnar Eigil (Intern)
Hotchkiss, Arland (Ekstern)
Søndergaard, Karen Marie (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Co-Combustion of Fossil Fuels and Waste

Department of Chemical and Biochemical Engineering
Period: 01/11/2007 → 21/09/2011
Number of participants: 7
Phd Student:
Wu, Hao (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Jappe Frandsen, Flemming (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Leckner, Bo (Ekstern)
Hupa, Mikko (Ekstern)
Hustad, Johan Einar (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD
Mathematical Modelling of Solid Oxide Fuel Cells
Department of Chemical and Biochemical Engineering
Period: 01/11/2007 → 13/04/2011
Number of participants: 8
Phd Student:
Mogensen, David (Intern)
Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Hendriksen, Peter Vang (Intern)
Nielsen, Jens Ulrik (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Jensen, Anker Degn (Intern)
Sehested, Jens (Intern)
Stimming, Ulrich (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Molecular Modelling of Protein Systems
Department of Chemical and Biochemical Engineering
Period: 01/11/2007 → 13/04/2011
Number of participants: 6
Phd Student:
Wedberg, Nils Hejle Rasmus Ingemar (Intern)
Supervisor:
Peters, Günther H.J. (Intern)
Main Supervisor:
Abildskov, Jens (Ekstern)
Examiner:
Hansen, Flemming Yssing (Intern)
Pleiss, Jürgen (Ekstern)
Rod, Thomas Holm (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Modeling and Experimental Investigation of Entrained-Flow Gasification of Biomass and Fossil Fuels
Department of Chemical and Biochemical Engineering
Period: 01/10/2007 → 11/05/2011
Number of participants: 6
Phd Student:
Brix, Jacob (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Wedel, Stig (Ekstern)
Leckner, Bo (Ekstern)
Pedersen, Lars Storm (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Ethanol Production from Rapeseed Straw and Agricultural Residues
Department of Chemical and Biochemical Engineering
Period: 15/09/2007 → 18/04/2012
Number of participants: 6
Phd Student:
Arvaniti, Efthalia (Intern)
Supervisor:
SLET - Kádár, Zsófia (Ekstern)
Main Supervisor:
Schmidt, Jens Ejbye (Intern)
Examiner:
Meyer, Anne S. (Intern)
Girio, Francisco M. Ferreira (Ekstern)
Norddahl, Birgir (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Katalytisk syntese af langkædedede alkoholer fra syntesegas fremstillet ved forgasning af kul og biomasse
Department of Chemical and Biochemical Engineering
Period: 15/09/2007 → 13/04/2011
Number of participants: 6
Phd Student:
Christensen, Jakob Munkholt (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Dahl, Søren (Ekstern)
Hinrichsen, Kai-Olaf (Ekstern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Gold Nanoparticles for Bladder Cancer Treatment
Department of Chemical and Biochemical Engineering
Period: 01/09/2007 → 24/11/2010
Number of participants: 5
Phd Student:
Javakhishvili, Irakli (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Szabo, Peter (Ekstern)
Galli, Giancarlo (Ekstern)
Jonsson, Eva E. Malmström (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Optimized Production of cement

Department of Chemical and Biochemical Engineering
Number of participants: 8
Phd Student:
Rasmussen, Martin Hagsted (Intern)
Supervisor:
Illerup, Jytte Boll (Intern)
Pedersen, Kim Hougaard (Intern)
Wedel, Stig (Ekstern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Jensen, Lars Skaarup (Intern)
Yrjas, Patrik Klaus (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Extension of Association Models to Complex Chemicals

Department of Chemical and Biochemical Engineering
Period: 01/08/2007 → 09/02/2011
Number of participants: 5
Phd Student:
Avlund, Ane Søgaard (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Hendriks, Eric M. (Ekstern)
Jackson, George (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD


Department of Chemical and Biochemical Engineering
Period: 15/07/2007 → 29/09/2010
Number of participants: 6
Phd Student:
Conte, Elisa (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Skov, Anne Ladegaard (Intern)
Continuous Membrane Microbioreactors for Development of Integrated Pectin Modification and Separation Processes

Department of Chemical and Biochemical Engineering
Period: 01/07/2007 → 09/02/2011
Number of participants: 7
Phd Student:
Zainal Alam, Muhd Nazrul Hisham Bin (Intern)
Supervisor:
Jonsson, Gunnar Eigil (Intern)
Meyer, Anne S. (Intern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Dufva, Martin (Intern)
Janssen, Anja E. M. (Ekstern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Flash Pyrolysis of Energy Crops

Department of Chemical and Biochemical Engineering
Period: 01/07/2007 → 21/11/2012
Number of participants: 5
Phd Student:
Ibrahim, Norazana (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Danne, Anne Juul (Intern)
Lundtorp, Kasper (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Integration of Modelling, Design and Control for Efficient Operation of chemical Processes

Department of Chemical and Biochemical Engineering
Period: 01/07/2007 → 13/04/2011
Number of participants: 6
Phd Student:
Abd Hamid, Mohd Kamaruddin Bin (Intern)
Supervisor:
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Manan, Zainuddin Abdul (Ekstern)
Skogestad, Sigurd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Migration of Plasticizers from PVC and Other Polymers
Department of Chemical and Biochemical Engineering
Period: 01/07/2007 → 09/02/2011
Number of participants: 7
Phd Student:
Lundsgaard, Rasmus (Intern)
Supervisor:
Aunskjaer, Ulrik (Ekstern)
Nielsen, Bjarne (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Hassager, Ole (Intern)
Mavrantzas, Vlasis G. (Ekstern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Modelling and Optimization of Integrated Bioreactor And Membrane Separation Processes
Department of Chemical and Biochemical Engineering
Period: 01/06/2007 → 24/11/2010
Number of participants: 6
Phd Student:
Prado Rubio, Oscar Andres (Intern)
Supervisor:
Jorgensen, Sten Bay (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Sorensen, Mads Peter (Intern)
Garde, Avid (Intern)
Wessling, Matthias (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

The Cloning and Expression of Lignocellulose Degrading Enzymes in Thermophilic Bacteria
Department of Chemical and Biochemical Engineering
Period: 01/05/2007 → 19/04/2013
Number of participants: 6
Phd Student:
Sitarz, Anna Katarzyna (Intern)
Lignocellulose Pretreatment for Lignin Removal and Maximal Enzymatic (Ligno) Cellulose Degradation

Department of Chemical and Biochemical Engineering
Period: 01/04/2007 → 01/09/2010
Number of participants: 7
Phd Student:
Pedersen, Mads (Intern)
Supervisor:
Johansen, Katja Salomon (Ekstern)
Pedersen, Sven (Ekstern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Jensen, Anker Degn (Intern)
Christensen, Morten Würtz (Ekstern)
Graff, Leendert H. de (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Oxy-fuel forbrænding af kul og biomasse

Department of Chemical and Biochemical Engineering
Period: 01/04/2007 → 24/08/2011
Number of participants: 8
Phd Student:
Toftegaard, Maja Bøg (Intern)
Supervisor:
Glarborg, Peter (Intern)
Jensen, Peter Arendt (Intern)
Sander, Bo (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Hupa, Mikko (Ekstern)
Jensen, Lars Skaarup (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD
Process-Product Synthesis, Design and Analysis through the Group- Contribution Approach

Department of Chemical and Biochemical Engineering
Period: 01/04/2007 → 01/09/2010
Number of participants: 7
Phd Student: Alvarado-Morales, Merlin (Intern)
Supervisor: Gernaey, Krist V. (Intern)
Woodley, John (Intern)
Main Supervisor: Gani, Rafiqul (Intern)
Examiner: Kontogeorgis, Georgios (Intern)
Camarda, Kyle V. (Ekstern)
Zondervan, Edwin (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Component-based Reactor Model of a Distillate Hydrotreater

Department of Chemical and Biochemical Engineering
Period: 15/03/2007 → 13/04/2011
Number of participants: 7
Phd Student: Boesen, Rasmus Risum (Intern)
Supervisor: Knudsen, Kim (Intern)
Michelsen, Michael Locht (Intern)
Main Supervisor: von Solms, Nicolas (Intern)
Examiner: Jensen, Anker Degn (Intern)
Christensen, Kurt Agerbæk (Ekstern)
Reimert, Rainer (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Enzymatic Opening of Diferulate Cross-Links in Plant Cell Walls

Department of Chemical and Biochemical Engineering
Period: 15/03/2007 → 15/06/2011
Number of participants: 6
Phd Student: Wittrup Agger, Jane (Intern)
Supervisor: Johansen, Katja Salomon (Ekstern)
Main Supervisor: Meyer, Anne S. (Intern)
Examiner: Woodley, John (Intern)
Biely, Peter (Ekstern)
Thomsen, Anne Belinda (Intern)

Financing sources
Development of Quantitative Kinetic Models Describing Enzyme Catalyzed Heteropolysaccaride Degradation: Soluble Arabinoxylan

Department of Chemical and Biochemical Engineering
Period: 01/03/2007 → 31/07/2010
Number of participants: 2
PhD Student:
Xu, Cheng (Intern)
Main Supervisor:
Meyer, Anne S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Kinetic Inhibition of Natural Gas Hydrates

Department of Chemical and Biochemical Engineering
Period: 01/03/2007 → 24/11/2010
Number of participants: 6
PhD Student:
Jensen, Lars (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Main Supervisor:
von Solms, Nicolas (Intern)
Examiner:
Michelsen, Michael Locht (Intern)
Herri, Jean-Michel (Ekstern)
Li, Xiaoyun (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Polymers for Insulin Reservoirs and Delivery Systems

Department of Chemical and Biochemical Engineering
Period: 01/03/2007 → 13/04/2011
Number of participants: 8
PhD Student:
Fristrup, Charlotte Juel (Intern)
Supervisor:
Jankova Atanasova, Katja (Intern)
Bukrinsky, Jens T. (Ekstern)
Eskimergen, Rüya (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Jonsson, Gunnar Eigil (Intern)
Buchmeiser, Michael R. (Ekstern)
Jørgensen, Lene (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet

Relations
Publications:
Polymers for Pharmaceutical Packaging and Delivery Systems
Project: PhD

Design of CO2 Capture Units using Aqueous Alkanolamines
Department of Chemical and Biochemical Engineering
Period: 15/02/2007 → 01/09/2010
Number of participants: 7
PhD Student:
Faramarzi, Leila (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Thomsen, Kaj (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Shapiro, Alexander (Intern)
Behrens, Paul K. (Ekstern)
van Well, Willy J. M. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of Quantitative Kinetic Models Describing Enzyme Catalysed Heteropolysaccharide Degradation: Insoluble Arabinoxylans
Department of Chemical and Biochemical Engineering
Period: 01/02/2007 → 15/06/2011
Number of participants: 6
PhD Student:
Rasmussen, Louise Enggaard (Intern)
Supervisor:
Sørensen, Jens Frisbak (Ekstern)
Main Supervisor:
Meyer, Anne S. (Intern)
Examiner:
Mikkelsen, Jern Dalgaard (Intern)
Pettersson, Dan Robert (Ekstern)
Tenkanen, Maija (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

High-Performance Anticorrosive Coatings
Department of Chemical and Biochemical Engineering
Period: 01/02/2007 → 04/06/2010
Number of participants: 7
PhD Student:
Sørensen, Per Aggerholm (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Multiphase Equilibrium in Systems with Production Chemicals

Department of Chemical and Biochemical Engineering
Period: 15/01/2007 → 30/09/2010
Number of participants: 5
Phd Student:
Fonseca, José (Intern)
Main Supervisor:
von Solms, Nicolas (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Richon, Dominique (Intern)
Solbraa, Even (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Biopolymer nanocomposite films and food packaging

Plastics produced from biodegradable polymers such as polylactide (PLA) are of increasing commercial interests. They are manufactured from renewable resources such as agricultural products and have the potential to meet environmental requirements.

However, a wider use of PLA in food packaging requires further material development in order to achieve the necessary stability and permeability profile to gas or water vapour. In the NanoPack project we will investigate improvement of PLA properties through nanoscale reinforcement using reinforcing fillers based on natural clay silicates and metal hydroxides.

The National Food Institute will characterise nanoparticles migrating from PLA film and perform in-vitro and in-vivo toxicological studies on relevant effect parameters. A thorough risk characterisation in the context of their use in food packaging will be performed by integrating results from exposure estimates and toxicological studies.

Project financing:
About 15 mio. DKK, with 50% from The Danish Research and Innovations Agency (DSF-NABIIT). The total budget for the National Food Institute is approximately 4.7 mio DKK.
**Evaluation of Prebiotic potential of novel carbohydrate preparations**

This project constitutes workpackage 2 in the 'Prebiotic Center, headed by Anne Meyer at DTU Chemical Engineering. The task of the Gut Ecology group at the National Food Institutes, Technical University of Denmark in the Center approach is to test for effects of novel carbohydrate preparations on the intestinal microbiota which may be relevant for human health. Specifically, we focus on the possibilities to prevent outbreaks of Ulcerative Colitis (UC).

We perform small-scale batch fermentations in pure cultures as well as in intestinal communities derived from healthy subjects and from subjects suffering from UC.

We analyse microbiota composition and metabolites produced by host and bacteria.

**Project financing:**
Danish Strategic Research Council
Øresund Food network
National Food Institute
Division of Food Microbiology
Department of Chemical and Biochemical Engineering

**Center for BioProcess Engineering**
Period: 01/01/2007 → 01/01/2013
Number of participants: 6
Acronym: Prebiotic potential of novel carbohydrate preparations
Number of related Ph.D. students: 1
Project participant:
- Vigsnæs, Louise Kristine (Intern)
- Holck, Jesper (Intern)
- Brynskov, Jørn (Ekstern)
- Steenholt, Carsten (Ekstern)
- Licht, Tine Rask (Intern)
- Phd Student:
- Sulek, Karolina (Intern)

**Mechanisms of Enzymatic Inactivation in the Animal Feed Pelleting Process**

Department of Chemical and Biochemical Engineering
Period: 01/01/2007 → 17/06/2010
Number of participants: 7
Phd Student:
- Puder, Katja (Intern)
- Supervisor:
- Jørgensen, Christian Isak (Ekstern)
- Simonsen, Ole (Ekstern)
- Main Supervisor:
- Jensen, Anker Degn (Intern)
- Examiner:
- Woodley, John (Intern)
- Hansen, Tomas T. (Ekstern)
- Lee, Geoffrey (Ekstern)

**Financing sources**
Source: Internal funding (public)
Renewable energy in the transport sector using biofuels as energy carriers

Biofuels, especially ethanol, have been in political focus for the last couple of years, both internationally and in Denmark. For the European Union, the EU Biofuel Directive has set a target of 5.75% by 2010 for the biofuel share of transport fuels. This has resulted in a couple of projects examining the impacts of biofuel introduction, by looking at individual production processes or lifecycle analyses of single technology applications. However, no detailed analyses of the nationwide implications in terms of changes in emissions, land use and other environmental effects have been undertaken to date. This project applies a scenario approach to investigate the abovementioned effects for Denmark. Three different transport fuel scenarios, a business-as-usual scenario, an EU policy scenario that adheres to the targets outlined in the EU Biofuel Directive and an impact-adapted scenario will be described. The impact-adapted scenario will incorporate the results of the two previous scenarios and outline a sustainable option for biofuel introduction in Denmark, taking into consideration and examining mitigation of, where possible, the negative implications for the environment and land use.

Department of Transport
Department of Chemical and Biochemical Engineering
Systems Analysis Division
Risø National Laboratory for Sustainable Energy
Aarhus University
Danish Technological Institute
Period: 01/01/2007 → 31/12/2010
Number of participants: 0
Acronym: REBECA

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 3,957,390.00 Danish Kroner

Teaching, Studying and Learning: Undersøgeæsæ af effekter og konsekvense af intensiv og aktiverende undervisning

Department of Civil Engineering
Office for Study Programmes and Student Affairs
Administration
Department of Mechanical Engineering
Department of Micro- and Nanotechnology
Department of Chemical and Biochemical Engineering
Department of Management Engineering
Period: 01/01/2007 → 31/03/2009
Number of participants: 5
Acronym: TeSt-Learn
Project participant:
Vigild, Martin Etchells (Intern)
Horsewell, Andy (Intern)
Thomsen, Erik Vilain (Intern)
Szabo, Peter (Intern)
Project Manager, organisational:
Christensen, Hans Peter (Intern)

Financing sources
Source: Uddannelse. Statslige. Andre statslige
Name of research programme: Uddannelse. Statslige. Andre statslige
Amount: 95,000.00 Danish Kroner
Workpackage 2 in Prebiotic Center: Gut microbiota and Immune Response Effects
The Prebiotic Center is a large research effort aiming to develop, synthesize and characterize new carbohydrates with beneficial effects on human health (e.g. prebiotics). This offers new possibilities for use of biological waste products. The Role of WP2 in Prebiotic Center is to reveal effects of putatively prebiotic carbohydrates on gut microbiota and immune function. We collaborate with Danisco and Herlev Hospital within this WP.

National Food Institute
Department of Chemical and Biochemical Engineering

Danisco AS
Period: 01/01/2007 → 31/12/2011
Number of participants: 9
Project participant:
Wilcks, Andrea (Intern)
Hemmingsen, Lene (Intern)
Vigsnæs, Louise Kristine (Intern)
Sulek, Karolina (Intern)
Brynskov, Jørn (Ekstern)
Steenholdt, Casper (Ekstern)
Lahtinen, Sampo (Ekstern)
Project Manager, organisational:
Licht, Tine Rask (Intern)
Meyer, Anne S. (Intern)

Nano-Scale Materials from Block Copolymers
Department of Chemical and Biochemical Engineering
Period: 15/11/2006 → 01/09/2010
Number of participants: 7
Phd Student:
Guo, Fengxiao (Intern)
Supervisor:
Jankova Atanasova, Katja (Intern)
Ndoni, Sokol (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Hvilsted, Søren (Intern)
Mortensen, Kell (Intern)
Tenhu, Heikki Juhani (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Physics of Adhesion
Department of Chemical and Biochemical Engineering
Period: 15/11/2006 → 17/03/2010
Number of participants: 7
Phd Student:
Keller, Mette Krog (Intern)
Supervisor:
Bach, Anders (Ekstern)
Skov, Anne Ladegaard (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Szabo, Peter (Ekstern)
Creton, Costantino (Ekstern)
Venerus, David C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Characterization of the Microfibrillar Structure of High Performance Polymer Materials
Department of Chemical and Biochemical Engineering
Period: 01/10/2006 → 10/02/2010
Number of participants: 8
Phd Student:
Pauw, Brian Richard (Intern)
Supervisor:
Andreasen, Jens Wenzel (Intern)
Klop, Enno A. (Ekstern)
Mortensen, Kell (Intern)
Main Supervisor:
Vigild, Martin Etchells (Intern)
Examiner:
Almdal, Kristoffer (Intern)
Fairclough, Patrick (Ekstern)
Hansen, Steen Laugesen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Data-driven Modelling for Monitoring and Control of Streptomyces Cultivations
Department of Chemical and Biochemical Engineering
Period: 01/10/2006 → 30/09/2010
Number of participants: 7
Phd Student:
Petersen, Nanna (Intern)
Supervisor:
Eliasson Lantz, Anna (Intern)
Stocks, Stuart M. (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
vanden Berg, Frans W.J. (Intern)
Glassey, Jarmila (Ekstern)
Haack, Martin Brian (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Co2 Injection in Low Permeable Oil and Gas Reservoir
Department of Chemical and Biochemical Engineering
Period: 15/09/2006 → 21/12/2010  
Number of participants: 6  
Phd Student: Niu, Ben (Intern)  
Supervisor: Stenby, Erling Halfdan (Intern)  
Yan, Wei (Intern)  
Main Supervisor: Shapiro, Alexander (Intern)  
Examiner: von Solms, Nicolas (Intern)  
Skauge, Arne (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD

Avanceret Reservoir Simulering  
Department of Chemical and Biochemical Engineering  
Period: 01/09/2006 → 24/11/2010  
Number of participants: 7  
Phd Student: Nielsen, Sidsel Marie (Intern)  
Supervisor: Michelsen, Michael Locht (Intern)  
Stenby, Erling Halfdan (Intern)  
Main Supervisor: Shapiro, Alexander (Intern)  
Examiner: Mosegaard, Klaus (Intern)  
Aavatsmark, Ivar (Ekstern)  
Jørgensen, Marianne (Intern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet  
Project: PhD

Model-Based Computer Aided Framework for Design of Process Monitoring and Analysis Systems  
Department of Chemical and Biochemical Engineering  
Number of participants: 6  
Phd Student: Singh, Ravendra (Intern)  
Supervisor: Gernaey, Krist V. (Intern)  
Main Supervisor: Gani, Rafiqul (Intern)  
Examiner: Woodley, John (Intern)  
Venkatasubramanian, Venkat (Ekstern)  
Wiebe, Lars (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD
Tilstopning af katalysatormonolitter i støvbelastede gasstrømme

Department of Chemical and Biochemical Engineering
Period: 01/09/2006 → 17/06/2010
Number of participants: 7
Phd Student:
Heiredal, Michael Lykke (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Jensen, Joakim Reimer (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Wedel, Stig (Ekstern)
Jensen, Jørgen Peter (Intern)
Mädler, Lutz (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Molecular Design using Grid Technology

Department of Chemical and Biochemical Engineering
Period: 01/06/2006 → 23/09/2009
Number of participants: 6
Phd Student:
Chelakara Satyanarayana, Kavitha (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Abildskov, Jens (Ekstern)
Examiner:
Kontogeorgis, Georgios (Intern)
Adjiman, Claire S. (Ekstern)
Camarda, Kyle V. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Continuous Culture Microbioreactors

Department of Chemical and Biochemical Engineering
Period: 01/05/2006 → 29/09/2010
Number of participants: 7
Phd Student:
Schäpper, Daniel (Intern)
Supervisor:
Eliasson Lantz, Anna (Intern)
Stocks, Stuart M. (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Woodley, John (Intern)
Duetz, Wouter A. (Ekstern)
Franco-Lara, Ezequiel (Ekstern)
**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

**NO Formation and destruction in the freeboard of Grate Boilers: CFD Model Development and Verification by Bench Scale Measurements**
Department of Chemical and Biochemical Engineering
Period: 01/04/2006 → 01/09/2010
Number of participants: 7
Phd Student:
Andersen, Jimmy (Intern)
Supervisor:
Hvid, Søren Lovmand (Ekstern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Hassager, Ole (Intern)
Eriksson, Jan Gunnar (Ekstern)
Løvås, Terese (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**In-Situ undersøgelser af forbrændingsprocesser i store to-takts dieselmotorer**
Department of Chemical and Biochemical Engineering
Period: 01/03/2006 → 17/03/2010
Number of participants: 7
Phd Student:
Poulsen, Hanne Hostrup (Intern)
Supervisor:
Clausen, Sønnik (Intern)
Mayer, Stefan (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Meyer, Knud Erik (Intern)
Rasmussen, Niels Bjarne Kampp (Ekstern)
Spicher, Ulrich (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

**Micro-sensor based on Click Chemistry**
Department of Chemical and Biochemical Engineering
Period: 01/03/2006 → 27/05/2009
Number of participants: 5
Phd Student:
Daugaard, Anders Egede (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Woodley, John (Intern)
Raman spectroscopy by use of UltraViolet Radiation: A new useful way to avoid fluorescence

Fluorescence has been a persistent problem in Raman spectroscopy. To avoid the problems a way to seems to have opened now: Excitation with deeply ultraviolet light. "Fluorescence does not appear to exist if the exciting light has a wavelength shorter than 260 nm" [cit.. S. A. Asher]. Affordable pulsed deep-UV lasers have recently been introduced to the market by a company "Photon Systems" in California. So-called HeAg og NeCu hollow-cathode lasers during operation create a metal vapor mixed with an inactive rare gas by a process reminding of sputtering. The lasers emit quasi-continuous laser light in the deep UV-range, with wavelengths of 224 nm (for silver) and 248 nm (for copper). During operation they require little electrical power and no water cooling. New instrument needed. We apply for a dedicated UV Raman-spectrometer with quartz optics, UV grating and detectors, and the necessary helping utensils. One important new aspect of the method is to introduce optical fibers, so that the optics can be totally encapsulated to avoid any deep UV radiation damage to objects and persons in the neighbourhood. UV-Raman spectroscopy will have many future applications. We will try the technique in three limited, well-defined research fields with a high content of new and innovative ideas. Hence, we want a new laser to abate fluorescence. We would like to use the new system in this way: 1) Characterisation of new waveguides by use of hollow microstructured crystal fibers. It ranges from analysis of Ge-nano-clusters embedded in silica-on-silicon planar waveguides to chemical and biological molecular identification. Samples will be prepared and investigated to find better methods to prepare silica materials with enhanced third order nonlinearity. Size and distribution of the nano-clusters are important parameters. In contrast to other methods, UV-Raman spectroscopy
needs no specimen preparation and should be a non-destructive, efficient method to find the size distribution of even very small nano-clusters. The UV Raman will be tried using hollow micro-structured optical fibers. Such air-hole fibers should enable easy and safe UV spectroscopy. This entirely new concept will be tried as well as fibers designed such that the air holes are used both for light guiding and at the same time as pipettes for a chemical solution (like gasoline/methanol mixtures) that one wants to analyse (co-work with COM-center). 2) Characterisation of fluorescing crude oil mixtures to help easy production and less pollution. Polycyclic aromatic hydrocarbons (PAHs) are highly intensive and characteristic Raman scatterers. Even small amounts (ppm to ppb scale or less) should be detectable (co-work with IVC-SEP-center). 3) Characterisation of biological and consumer samples, where fluorescence is a problem. Organic molecules, e.g. proteins, nucleic acids (DNA), hormones, phthalates and pigments in the household and other environments should exhibit Raman and resonance Raman spectra with a lot of information on structure and function if only the fluorescence could be avoided. We will try this by a study of insuline in living tissue (distribution, structure and other characterisations). Also we will start on the obvious project of cancer cell characterisation (a co-work with the QUP-center). 4) We are also studying pigments and objects from the Ny Carlsberg Glyptotek. The intention is to set the UV Raman instrument up, and then carry out the subprojects 1) - 4) simultaneously. The ph.d. project will have the complete set of subprojects as its objective, but parts of the work are to be done even without a ph.d.-salary.

Department of Chemistry

Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

Period: 01/01/2006 → 01/01/2009
Number of participants: 1
Acronym: UVRS
Project Manager, organisational:
Søtofte, Inger (Intern)

Financing sources
Source: Uddannelse, udenlandske offentlige og private
Name of research programme: Uddannelse, udenlandske offentlige og private
Amount: 10,000.00 Danish Kroner

New Plastics and Processes for Disposable Delivery Systems

Department of Chemical and Biochemical Engineering

Period: 15/12/2005 → 24/06/2009
Number of participants: 10
Phd Student:
Laursen, Jens Lolle (Ekstern)
Supervisor:
Brøndsted, Povl (Intern)
Christoffersen, Lasse Wengel (Intern)
Horsewell, Andy (Intern)
Papøe, Mogens (Ekstern)
Sivebæk, Ion Marius (Intern)
Main Supervisor:
Vigild, Martin Etchells (Intern)
Examiner:
Hansen, Hans Nørgaard (Intern)
Andreassen, Erik (Intern)
Vejen, Nikolaj Conradsen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Application of Force Field Enhanced Filtration to the Recovery of Biological Products

Department of Chemical and Biochemical Engineering

Period: 01/12/2005 → 14/12/2007
Number of participants: 4
Phd Student:
Controlled Release of Environmentally Friendly Antifouling Agents from Marine Coatings

Department of Chemical and Biochemical Engineering
Period: 01/11/2005 → 01/04/2009
Number of participants: 7
PhD Student:
Olsen, Stefan Møller (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Pedersen, Lars Thorslund (Intern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Woodley, John (Intern)
Swain, Geoffrey W. (Ekstern)
Erik Weinell, Claus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Development of Group Contribution plus Models for Properties of Organic Chemical Systems

Department of Chemical and Biochemical Engineering
Period: 01/10/2005 → 26/08/2009
Number of participants: 6
PhD Student:
Gonzalez Villalba, Hugo Edson (Intern)
Supervisor:
Abildskov, Jens (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Cisneros, Eduardo Salvador P. (Intern)
Schiller, Martin (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Molecular Design using GRID Technology

Department of Chemical and Biochemical Engineering
Programkomitéen for nanovideneskab og teknologi
Period: 01/10/2005 → 30/09/2008
Number of participants: 1
Project participant:
Abildskov, Jens (Ekstern)

Financial sources
Source: Forsk. EU - Andre EU-midler
Name of research programme: Forsk. EU - Andre EU-midler
Amount: 2,216,329.20 Danish Kroner

Pre-Treatment (and Enzymatic Hydrolysis) of Ligno-Cellulose
Department of Chemical and Biochemical Engineering
Period: 01/10/2005 → 21/12/2010
Number of participants: 7
Phd Student:
Andric, Pavle (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Meyer, Anne S. (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Viladsen, John (Intern)
Lidén, Gunnar (Ekstern)
Olsen, Hans Sejr (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Module Design and Performance in Microfiltration, Ultrafiltration and Membrane Contactors
Department of Chemical and Biochemical Engineering
Period: 01/09/2005 → 19/12/2008
Number of participants: 5
Phd Student:
Beier, Søren (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Woodley, John (Intern)
Aimar, Pierre (Ekstern)
Kristensen, Steen (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Process for Recovering and Enzymatically Modifying Immuno-Modulating Lipoteichoic Acid from Industrial Bacillus Fermentations
Department of Chemical and Biochemical Engineering
Period: 01/09/2005 → 28/02/2007
Number of participants: 4
Phd Student:
Hua, Ling (Intern)
Supervisor:
Upscaling of Particulate Processes in Fluidised Beds

Department of Chemical and Biochemical Engineering
Period: 01/09/2005 → 30/01/2009
Number of participants: 6
Phd Student:
Hede, Peter Dybdahl (Intern)
Supervisor:
Bach, Poul (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Hansen, Tomas T. (Ekstern)
Seville, Jonathan P. K. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Molecular Modelling of Polymer Melt Rheology

Department of Chemical and Biochemical Engineering
Period: 15/08/2005 → 29/04/2009
Number of participants: 7
Phd Student:
Wang, Yanwei (Intern)
Supervisor:
Hansen, Flemming Yssing (Intern)
Peters, Günther H.J. (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Shapiro, Alexander (Intern)
Vlassopoulos, Dimitrios (Intern)
de Pablo, Juan J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Particle Formation in Natural Gas Combustion

Department of Chemical and Biochemical Engineering
Period: 15/08/2005 → 01/04/2009
Number of participants: 7
Phd Student:
Wagner, Ayten Yilmaz (Intern)
Center for Individual Nanoparticle Functionality
The main objective of the centre is to explore and understand the fundamental relations between surface morphology and reactivity on the nanometer scale. A combination of new experimental initiatives supported by theoretical approaches will be employed. The primary objectives of the center are: * To establish a close and unambiguous correlation between the morphology and the reactivity, ultimately of experimental approaches and methods. * To challenge the widely held belief that there are chemical reactions catalyzed by metal surfaces, which are structure insensitive, i.e. without a strong dependence on the detailed atomic structure of the surface. * To develop a new concept where nanodstructures can catalyze chemical reactions under non-thermal conditions, operating on entirely different physical principles than current technology.

Experimental Surface and Nanomaterials Physics

Department of Physics
Department of Micro- and Nanotechnology
Department of Chemical and Biochemical Engineering
Center for Individual Nanoparticle Functionality
Haldor Topsoe AS
Technical University of Munich
Eindhoven University of Technology
Chalmers University of Technology
Period: 01/08/2005 → 31/07/2010
Number of participants: 5
Acronym: CINF
Project ID: 20211
Project participant:
Nielsen, Jane Hvolbæk (Intern)
Quaade, Ulrich (Intern)
Schietz, Jakob (Intern)
Hansen, Ole (Intern)
Project Manager, organisational:
Chorkendorff, Ib (Intern)

Financing sources
Source: Forsk. Andre statslige danske - Grundforskn.fonden
Name of research programme: Forsk. Andre statslige danske - Grundforskn.fonden
Amount: 36,000,000.00 Danish Kroner
Project

Computer-Aided Product Design using the PC-SAFT Equation of State
Department of Chemical and Biochemical Engineering
Period: 01/06/2005 → 25/09/2008
Number of participants: 7
Phd Student:
Tihic, Amra (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
von Solms, Nicolas (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Thomsen, Kaj (Intern)
Dahl, Søren (Ekstern)
Hemptinne, Jean-Charles de (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Stabilisering af Polyethylenglycol i Arkæologisk Træ

Department of Chemical and Biochemical Engineering
Period: 01/06/2005 → 01/04/2009
Number of participants: 6
Phd Student:
Mortensen, Martin Nordvig (Intern)
Supervisor:
Glastrup, Jens (Ekstern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Jonsson, Gunnar Eigil (Intern)
Eiding, Lars I. (Ekstern)
Jones, Mark (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Development of Derivatized Hyaluronic Acid and Formulation of Nanocapsules for Delivery of Cosmetic Actives and Pharmaceutical Drugs

Department of Chemical and Biochemical Engineering
Period: 15/05/2005 → 03/11/2008
Number of participants: 9
Phd Student:
Eenschooten, Corinne Diane (Intern)
Supervisor:
Gurny, Robert (Ekstern)
Guillaumie, Fanny (Intern)
Schwach-Abdellaoui, Khadija (Ekstern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Almdal, Kristoffer (Intern)
Allémann, Éric (Ekstern)
Guy, Richard H. (Ekstern)

Financing sources
Source: Internal funding (public)
Fremstilling af Asymmetriske Membraner ved Deponering af Nano-Partikler
Department of Chemical and Biochemical Engineering
Period: 01/03/2005 → 29/08/2008
Number of participants: 7
Phd Student:
Elmøe, Tobias Dokkedal (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Pratsinis, Sotiris E. (Ekstern)
Main Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Examiner:
Jonsson, Gunnar Eigil (Intern)
Clausen, Bjerne S. (Intern)
Mädler, Lutz (Ekstern)

Financing sources
Source: Internal funding (public)

Gypsum Crystallisation and Foaming Prevention in Wet Flue Gas Desulphurization (FGD) Plants
Department of Chemical and Biochemical Engineering
Period: 01/03/2005 → 27/10/2008
Number of participants: 6
Phd Student:
Hansen, Brian Brun (Intern)
Supervisor:
Johnsson, Jan Erik (Intern)
Main Supervisor:
Küll, Søren (Intern)
Examiner:
Wedel, Stig (Ekstern)
Karlstson, Hans T. (Ekstern)
Kristensen, Nicholas (Ekstern)

Financing sources
Source: Internal funding (public)

Design of Fibre Surfaces used in Composites
Department of Chemical and Biochemical Engineering
Period: 01/02/2005 → 25/09/2008
Number of participants: 8
Phd Student:
Drews, Joanna Maria (Intern)
Supervisor:
Almdal, Kristoffer (Intern)
Kingshott, Peter (Intern)
West, Keld (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Model Identification for Predictive Control and Optimization

Department of Chemical and Biochemical Engineering
Period: 01/02/2005 → 24/11/2008
Number of participants: 6
Phd Student:
Huusom, Jakob Kjøbsted (Intern)
Supervisor:
Poulsen, Niels Kjølstad (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Jørgensen, John Bagterp (Intern)
Andersen, Henrik Weisberg (Ekstern)
Bombois, Xavier (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Nano-Porous Materials from Self-Organizing Soft Matter

Department of Chemical and Biochemical Engineering
Period: 01/02/2005 → 01/07/2009
Number of participants: 7
Phd Student:
Szewczykowski, Piotr Przemyslaw (Intern)
Supervisor:
Berg, Rolf Henrik (Intern)
Ndoni, Sokol (Intern)
Main Supervisor:
Vigild, Martin Etchells (Intern)
Examiner:
Almdal, Kristoffer (Intern)
Jannasch, Patric (Ekstern)
Posselt, Dorthe (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-lønnet stipendie
Project: PhD

Prediction of Wine Quality from Phenolic Profiles of Grapes, forkortet “Wine Quality”

Department of Chemical and Biochemical Engineering
Period: 01/02/2005 → 04/07/2008
Number of participants: 6
Phd Student:
Jensen, Jacob Skibsted (Intern)
Supervisor:
Design of functional nanomaterials
To establish a research collaboration encompassing all steps in the development of new functional nanomaterials: design, synthesis, characterization, and testing. The common aim of the proposal is the development of rational design strategies for nano-structured materials.

Department of Physics
Department of Chemistry
Administration
Department of Chemical and Biochemical Engineering
Department of Micro- and Nanotechnology
Risø National Laboratory for Sustainable Energy
Center for Individual Nanoparticle Functionality

Center for Nanoteknologi
Period: 01/01/2005 → 31/12/2008
Number of participants: 19
Project ID: 20195
Project participant:
Jacobsen, Karsten Wedel (Intern)
Chorkendorff, Ib (Intern)
Nielsen, Jane Hvolbæk (Intern)
Horch, Sebastian (Intern)
Schietz, Jakob (Intern)
Hansen, Jern Bindslev (Ekstern)
Quaade, Ulrich (Intern)
Christensen, Claus H. (Intern)
Ulstrup, Jens (Intern)
Johannessen, Tue (Intern)
Bøggild, Peter (Intern)
Pedersen, Allan Schröder (Intern)
Linderoth, Søren (Intern)
Mogensen, Mogens (Intern)
Vegge, Tejs (Intern)
Pryds, Nini (Intern)
Henriksen, Peter Vang (Ekstern)
Kuhn, Luise Theil (Intern)
Project Manager, organisational:
Nørskov, Jens Kehlet (Intern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 9,290,000.00 Danish Kroner
**Heterogeneous catalysis for chemical production**
Catalysis is one of the technological pillars of modern chemical industry. Catalysis also holds the key to the solution of many environmental and energy problems. The challenge in the field is to devise new methods that can accelerate the development of new catalysts and processes beyond the intuitive trial-and-error approach. It is suggested to form a collaborative program encompassing the whole range from computational design and experimental analysis of model systems to synthesis and testing of new catalysts. The aim of the program is to develop new tools allowing for the rational design of catalysts and catalytic processes for chemical industry and for environmental protection.

Department of Physics
Department of Chemistry
Department of Chemical and Biochemical Engineering
Center for Nanoteknologi
Haldor Topsoe AS
University of Iceland
Period: 01/01/2005 → 31/12/2009
Number of participants: 5
Project ID: 20194
Project participant:
Horch, Sebastian (Intern)
Christensen, Claus H. (Intern)
Johannessen, Tue (Intern)
Jonsson, Hannes (Ekstern)
Project Manager, organisational:
Nørskov, Jens Kehlet (Ekstern)

**Financing sources**
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 14,000,000.00 Danish Kroner

**New electrode materials for hydrogen production**
It is proposed to explore the potential of a recent invention where a new class of materials has been identified as electrodes for hydrogen evolution. Presently platinum and other extremely expensive noble metals are the best electrode materials, and it is essential for a possible future hydrogen economy to find cheaper and equally efficient replacements. Our approach involves a search for new and more efficient variations of a new class of materials based on transition metal sulfides. We will be exploiting the synergy between designs on the basis of electronic structure calculations and the synthesis and testing of new materials.

Department of Physics
Department of Chemical and Biochemical Engineering
Center for Individual Nanoparticle Functionality
IRD Fuel Cells A/S
Period: 01/01/2005 → 31/12/2007
Number of participants: 1
Project ID: 20197
Project Manager, organisational:
Chorkendorff, Ib (Intern)

**Financing sources**
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 3,600,000.00 Danish Kroner
Deactivation of SCR Catalysts by Additives
Department of Chemical and Biochemical Engineering
Period: 01/12/2004 → 19/12/2008
Number of participants: 7
Phd Student: Castellino, Francesco (Intern)
Supervisor: Fehrmann, Rasmus (Intern)
Johnsson, Jan Erik (Intern)
Main Supervisor: Jensen, Anker Degn (Intern)
Examiner: Grunwaldt, Jan-Dierk (Intern)
Pedersen, Henrik Guldberg (Intern)
Sander, Bo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Reactivity and Burnout of Wood Fuels
Department of Chemical and Biochemical Engineering
Period: 01/12/2004 → 14/12/2011
Number of participants: 6
Phd Student: Dall'Ora, Michelangelo (Intern)
Supervisor: Jensen, Peter Arendt (Intern)
Main Supervisor: Jensen, Anker Degn (Intern)
Examiner: Glarborg, Peter (Intern)
Jensen, Jørgen Peter (Intern)
Skreiberg, Øyvind (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

CHIGP BP
Funded by BP
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 05/11/2004 → 31/12/2013
Number of participants: 1
Project ID: 50357
Project Manager, academic: Kontogeorgis, Georgios (Intern)

Modelling and Design of Chemically Formulated Products
Department of Chemical and Biochemical Engineering
Design of an All-Polymer Micro Pump

Department of Chemical and Biochemical Engineering
Period: 01/10/2004 → 25/03/2008
Number of participants: 6
Phd Student:
Hansen, Thomas Steen (Intern)
Supervisor:
Larsen, Niels Bent (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Bechgaard, Klaus (Intern)
Wegner, Gerhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Flashpyrolyse af Halm in Situ

Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 29/08/2008
Number of participants: 6
Phd Student:
Bech, Niels (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Wedel, Stig (Ekstern)
Hustad, Johan Einar (Ekstern)
Madsen, Ole Hedegaard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: InnovationsPhD
Project: PhD
History Matching using Stochastic Methods
Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 15/05/2008
Number of participants: 6
Phd Student:
Johansen, Kent (Ekstern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Michelsen, Michael Locht (Intern)
Hu, Lin Y. (Ekstern)
Mosegaard, Klaus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Influence of Formulation in Formation of Enzyme Granules by Spray Drying
Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 28/01/2007
Number of participants: 7
Phd Student:
Sloth, Jakob (Intern)
Supervisor:
Bach, Poul (Ekstern)
Jensen, Anker Degn (Intern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Woodley, John (Intern)
Hansen, Tomas T. (Ekstern)
Seville, Jonathan P. K. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Preparation of Amphiphilic, Functionalised Copolymers for Coatings, Matrics and Adhesives
Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 01/04/2009
Number of participants: 7
Phd Student:
Overgaard, Anne Kathrine Kattenhøj (Intern)
Supervisor:
Everland, Hanne (Ekstern)
Vange, Jakob (Ekstern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Szabo, Peter (Ekstern)
Bock, Klaus (Ekstern)
Jonsson, Eva E. Malmström (Ekstern)
**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

**Produktion af lægemidler**
Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 25/02/2008
Number of participants: 7
Phd Student:
Christensen, Henrik (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Nielsen, Ole (Ekstern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Buchwald, Stephen L. (Ekstern)
Dancer, Robert J. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet

**Relations**
Publications:
Analysis of a Buckwald-Hartwig amination: reaction for pharmaceutical production
Analysis of a Buchwald-Hartwig amination: reaction for pharmaceutical production
Project: PhD

**Avanceret Reservoirsimulering**
Department of Chemical and Biochemical Engineering
Period: 15/08/2004 → 16/05/2008
Number of participants: 7
Phd Student:
Kristensen, Morten Rode (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Thomsen, Per Grove (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Shapiro, Alexander (Intern)
Aavatsmark, Ivar (Ekstern)
Saaf, Fredrik (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**Physical Properties of Complex Chemical Systems**
Department of Chemical and Biochemical Engineering
Period: 01/08/2004 → 29/08/2008
Number of participants: 5
Phd Student:
Christensen, Steen (Intern)
Main Supervisor:
Abildskov, Jens (Ekstern)
Examiner:
Møller, Klaus Braagaard (Intern)
Martin, Marcus G. (Ekstern)
Schiller, Martin (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Samtidig måling af lydhastighed og elektrisk ledningsevne af sedimenter som funktion af spændingstilstand og væskemætning.
Bevillingen er givet til anskaffelse af nyt apparatur, som monteres i eksisterende triaxialt trykapparat, således at målingerne udføres ved trykbetingelse svarende til reservoires tryk.

Department of Environmental Engineering
Department of Chemical and Biochemical Engineering
Period: 01/08/2004 → 01/06/2005
Number of participants: 3
Acronym: 441
Project ID: 30345
Project participant:
Olsen, Casper (Intern)
Stenby, Erling (Ekstern)
Project Manager, organisational:
Fabricius, Ida Lykke (Intern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 357,600.00 Danish Kroner
Project

Design af Emulsioner
Department of Chemical and Biochemical Engineering
Period: 01/07/2004 → 16/05/2008
Number of participants: 5
Phd Student:
Egholm, Runi Ditlev (Intern)
Main Supervisor:
Szabo, Peter (Intern)
Examiner:
Rasmussen, Henrik K. (Intern)
Harlen, Oliver Guy (Ekstern)
Trägårdh, Christian (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Udvikling af integrerede DMFC & PEM brænsecelle enheder : (PSO-projekt)
Department of Chemical and Biochemical Engineering
IRD Fuel Cells A/S
Aalborg University
University of Southern Denmark  
**Period:** 01/06/2004 → 01/06/2007  
**Number of participants:** 2  
**Project participant:**  
Johannessen, Tue (Intern)  
Chorkendorff, Ib (Intern)  

**Financing sources**  
Source: Forsk. Andre statslige danske i øvrigt  
Name of research programme: Forsk. Andre statslige danske i øvrigt  
Amount: 1,503,000.00 Danish Kroner  

**Project**  
Post-translational Modifications of Proteins: Novel in Vitro Methods for their Study and Scale-up  
Department of Chemical and Biochemical Engineering  
**Period:** 01/04/2004 → 25/06/2007  
**Number of participants:** 7  
Phd Student:  
Maury, Trine Lütken (Intern)  
**Supervisor:**  
Brask, Jesper (Intern)  
Hobley, Timothy John (Intern)  
Main Supervisor:  
Villadsen, John (Intern)  
Examiner:  
Meyer, Anne S. (Intern)  
Franzreb, Matthias (Ekstern)  
Friedmann, Thomas (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU, Samfinansiering  

**Recycling of Alkali in bio fly ash**  
Center for Phase Equilibria and Separation Processes  
Department of Chemical and Biochemical Engineering  
**Period:** 01/04/2004 → 31/12/2005  
**Number of participants:** 1  
**Project Manager, organisational:**  
Thomsen, Kaj (Intern)  

**Financing sources**  
Source: Sam.arb.aftaler, Private danske - Andre virksomheder  
Name of research programme: Sam.arb.aftaler, Private danske - Andre virksomheder  
Amount: 1,000,000.00 Danish Kroner  

**Development of Berry Fruit Juices with Improved Health Potential**  
Department of Chemical and Biochemical Engineering  
**Period:** 15/03/2004 → 25/11/2009  
**Number of participants:** 5  
Phd Student:  
Arnous, Anis (Intern)  
Main Supervisor:  
Meyer, Anne S. (Intern)  
Examiner:
Mikkelsen, Jørn Dalgaard (Intern)
Dietrich, Helmut (Ekstern)
vanden Brink, Hans (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Måling af fysisk-kemiske egenskaber for calcium-natrium iminodisulphonat trihydrat - Ca-Na[N(SO3)2]∙3H2O
Department of Chemical and Biochemical Engineering
Elsam A/S
Period: 01/03/2004 → 31/05/2004
Number of participants: 1
Project Manager, organisational:
Thomsen, Kaj (Intern)

Financing sources
Source: Sam.arb.aftaler, Private danske - Andre virksomheder
Name of research programme: Sam.arb.aftaler, Private danske - Andre virksomheder
Amount: 213,904.00 Danish Kroner
Project

Partial Oxidation of Natural Gas to Liquid Fuels
Department of Chemical and Biochemical Engineering
Period: 15/02/2004 → 26/10/2007
Number of participants: 5
PhD Student:
Rasmussen, Christian Lund (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Villadsen, John (Intern)
Alzueta, Maria (Intern)
Østberg, Martin (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Conflict-based Method for Economical, Substainable, Safe and Environmentally Clean Process (Retrofit) Design and Operation
Department of Chemical and Biochemical Engineering
Period: 01/02/2004 → 25/09/2008
Number of participants: 6
PhD Student:
Davidescu, Florin Paul (Intern)
Supervisor:
Madsen, Henrik (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Kristensen, Niels Rode (Intern)
Marquardt, Wolfgang (Ekstern)

Financing sources
Corrosion in Wet Gas Pipelines
Department of Chemical and Biochemical Engineering
Period: 01/02/2004 → 25/03/2008
Number of participants: 6
Phd Student:
Fosbøl, Philip Loldrup (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Mollerup, Jørgen (Intern)
Dugstad, Arne (Ekstern)
Rislund, Ebbe (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Emission fra cement produktion
Department of Chemical and Biochemical Engineering
Period: 01/02/2004 → 30/04/2007
Number of participants: 7
Phd Student:
Hu, Guilin (Intern)
Supervisor:
Hansen, Jens Peter (Intern)
Wedel, Stig (Ekstern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Kiil, Søren (Intern)
Hupa, Mikko (Ekstern)
Jensen, Lars Skaarup (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Rheology, Structural Studies and Synthesis
Department of Chemical and Biochemical Engineering
Period: 01/02/2004 → 29/08/2007
Number of participants: 7
Phd Student:
Nielsen, Jens Kromann (Intern)
Supervisor:
Almdal, Kristoffer (Intern)
Mortensen, Kell (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Development of New Synthetic Membranes for Use in Micro Glucose Sensors

Department of Chemical and Biochemical Engineering
Period: 01/01/2004 → 03/09/2007
Number of participants: 6
Phd Student: Hansen, Natanya Majbritt Louie (Intern)
Supervisor: Gerstenberg, Michael Christian (Intern)
Main Supervisor: Hvilsted, Søren (Intern)
Examiner: Jonsson, Gunnar Eigil (Intern)
Galli, Giancarlo (Ekstern)
Jannasch, Patric (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Kompositter som lavfrikstions materialer

Department of Chemical and Biochemical Engineering
Period: 01/01/2004 → 20/06/2007
Number of participants: 6
Phd Student: Larsen, Thomas Ricco Ølholm (Intern)
Supervisor: Løgstrup Andersen, Tom (Intern)
Main Supervisor: Vigild, Martin Etchells (Intern)
Examiner: Szabo, Peter (Ekstern)
Friedrich, Klaus (Ekstern)
Sivebæk, Ion Marius (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

CO2 Capture from Coal Fired Power Plants

Department of Chemical and Biochemical Engineering
Period: 01/11/2003 → 16/02/2007
Number of participants: 7
Phd Student: Gabrielsen, Jostein (Intern)
Supervisor: Kontogeorgis, Georgios (Intern)
Modelling of Complex Mixtures Containing Hydrogen Bonding Molecules using CPA EOS

Department of Chemical and Biochemical Engineering
Period: 01/11/2003 → 22/01/2007
Number of participants: 7
Phd Student: Folas, Georgios (Intern)
Supervisor: Michelsen, Michael Locht (Intern)
Main Supervisor: Kontogeorgis, Georgios (Intern)
Examiner: Abildskov, Jens (Ekstern)
Economou, Ioannis (Intern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Forbrændingsmekanismer ved udnyttelse af affald som brændsel i cementproduktion

Department of Chemical and Biochemical Engineering
Period: 01/10/2003 → 30/04/2007
Number of participants: 8
Phd Student: Larsen, Morten Boberg (Intern)
Supervisor: Jappe Frandsen, Flemming (Intern)
Glarborg, Peter (Intern)
Jensen, Lars Skaarup (Intern)
Main Supervisor: Dam-Johansen, Kim (Intern)
Examiner: Livbjerg, Hans (Intern)
Høstgaard-Jensen, Jesper (Ekstern)
Leckner, Bo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Laboratorieundersøgelse af aerosoldannelse og kemiske reaktioner i ræggas fra biomasse- og affaldsforbrænding
Department of Chemical and Biochemical Engineering

Period: 01/10/2003 → 20/06/2007
Number of participants: 7
Phd Student:
Zeuthen, Frederik Jacob (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Glarborg, Peter (Intern)
Main Supervisor:
Livbjerg, Hans (Intern)
Examiner:
Johnsson, Jan Erik (Intern)
Ballester, Javier (Ekstern)
Pedersen, Lars Storm (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Chemistry and Computational Fluid Dynamics

Department of Chemical and Biochemical Engineering
Period: 01/09/2003 → 01/04/2004
Number of participants: 3
Phd Student:
Christensen, Mikkel Stochkendahl (Intern)
Supervisor:
Jensen, Anker Degn (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Development of an Equation of State to Solutions Containing Electrolytes

Department of Chemical and Biochemical Engineering
Period: 01/09/2003 → 03/09/2007
Number of participants: 5
Phd Student:
Lin, Yi (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Mollerup, Jørgen (Intern)
Fürst, Walter (Ekstern)
Jensen, Jørgen Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Fotodimerisering i peptider til optisk lagring

Department of Chemical and Biochemical Engineering
Period: 01/09/2003 → 30/04/2007
Number of participants: 7
Phd Student:
Lohse, Brian (Ekstern)
Supervisor:
Berg, Rolf Henrik (Intern)
Ramanujam, P.S. (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Vigild, Martin Etchells (Intern)
Jonsson, Eva E. Malmström (Ekstern)
Matharu, Avtar Singh (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Len)
Project: PhD

Gas-phase Sulfur, Chlorine and Alkali Metal Chemistry in Biomass Combustion
Department of Chemical and Biochemical Engineering
Period: 01/09/2003 → 03/09/2007
Number of participants: 7
Phd Student:
Løj, Lusi Hindiyarti (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Livbjerg, Hans (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Jensen, Peter Arendt (Intern)
Hupa, Mikko (Ekstern)
Kristensen, Per Graves (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Modelling for Monitoring, Control and Optimization of Fed-Batch
Department of Chemical and Biochemical Engineering
Period: 01/09/2003 → 02/06/2008
Number of participants: 7
Phd Student:
Rasmussen, Jan Kamyno (Intern)
Supervisor:
Jørgensen, Henrik Steen (Ekstern)
Madsen, Henrik (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Lei, Frede (Intern)
Lübbert, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
**Stability of Enzymes in Granular Enzyme Products for Laundry Detergents**

Department of Chemical and Biochemical Engineering  
Period: 01/09/2003 → 01/09/2010  
Number of participants: 8  
Phd Student:  
Biran, Suzan (Intern)  
Supervisor:  
Bach, Poul (Ekstern)  
Kil, Søren (Intern)  
Simonsen, Ole (Ekstern)  
Main Supervisor:  
Jensen, Anker Degn (Intern)  
Examiner:  
Mikkelsen, Jørn Dalgaard (Intern)  
Cedervall, Tommy (Ekstern)  
Hansen, Tomas T. (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU, Samfinansiering

**Relations**  
Publications:  
Stability of Enzymes in Granular Enzyme Products for Laundry Detergents  
Project: PhD

**CHIGP Statoil**  
Funded by Statoil  
Center for Energy Resources Engineering  
Department of Chemical and Biochemical Engineering  
CERE – Center for Energy Resources Engineering  
Period: 03/07/2003 → 31/12/2014  
Number of participants: 1  
Project ID: 50264  
Project Manager, academic:  
Kontogeorgis, Georgios (Intern)  

**Enzymatisk Hydrolyse af Lignocellulose fra Byg, Strå og Skaller**  
Department of Chemical and Biochemical Engineering  
Number of participants: 6  
Phd Student:  
Rosgaard, Lisa (Ekstern)  
Supervisor:  
Pedersen, Sven (Ekstern)  
Main Supervisor:  
Meyer, Anne S. (Intern)  
Examiner:  
Villadsen, John (Intern)  
Nielsen, Charles (Ekstern)  
Tjerneld, Folke (Ekstern)  

**Financing sources**
Nanomaterialer til hydro-/dehydrogeneringsreaktioner

Department of Chemical and Biochemical Engineering
Period: 01/07/2003 → 12/12/2008
Number of participants: 7
Phd Student:
Rovik, Anne (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Grunwaldt, Jan-Dierk (Intern)
Herbst, Konrad (Ekstern)
Olsbye, Unni (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Experimental Studies and Modeling of Asphaltene Precipitation Caused by Gas Injection

Department of Chemical and Biochemical Engineering
Period: 01/05/2003 → 01/09/2006
Number of participants: 6
Phd Student:
Verdier, Sylvain Charles Roland (Intern)
Supervisor:
Ivar Andersen, Simon (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Lindeloff, Niels (Intern)
Randzio, Stanislaw L. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

Alloy Catalyst for Direct Methanol Fuel Cells

Department of Chemical and Biochemical Engineering
Period: 01/04/2003 → 15/09/2006
Number of participants: 7
Phd Student:
Chakraborty , Debasish (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Livbjerg, Hans (Intern)
Main Supervisor:
Johannessen, Tue (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Skou, Eivind Morten (Ekstern)
Yde-Andersen, Steen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lænnet stipendie
Project: PhD

Aktivering af Metan ved Partiel Oxidation i Katalytisk Membranreaktor
Department of Chemical and Biochemical Engineering
Period: 01/02/2003 → 28/08/2006
Number of participants: 6
Phd Student:
Johansen, Johnny (Ekstern)
Supervisor:
Livbjerg, Hans (Intern)
Main Supervisor:
Johannessen, Tue (Intern)
Examiner:
Jonsson, Gunnar Eigil (Intern)
Nielsen, Michael Brorson (Intern)
Pratsinis, Sotiris E. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Computer Aided Modelling for Bio- and Chemical, Process/Product Design
Department of Chemical and Biochemical Engineering
Period: 01/12/2002 → 30/05/2006
Number of participants: 5
Phd Student:
Sales Cruz, Alfonso Mauricio (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Cisneros, Eduardo Salvador P. (Intern)
Clement, Karsten (Intern)
Georgiadis, Michael C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Phase Behaviour and Viscosity Modelling of Refrigerants-Lubricants Mixtures
Department of Chemical and Biochemical Engineering
Period: 01/11/2002 → 30/03/2006
Number of participants: 6
Phd Student:
Monsalvo, Matias Alfonso (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Fremstilling og Karakterisering af nye Metalhydrid til Lagring af Brint

Department of Chemical and Biochemical Engineering
Period: 01/10/2002 → 07/03/2006
Number of participants: 8
Phd Student: Andreasen, Anders (Ekstern)
Supervisor: Besenbacher, Flemming (Intern)
Dahl, Søren (Intern)
Pedersen, Allan Schrøder (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)
Examiner: Jensen, Jens Oluf (Intern)
Fichtner, Maximilian (Ekstern)
Züttel, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Modelling of Mineral Scale Deposition

Department of Chemical and Biochemical Engineering
Period: 01/10/2002 → 22/12/2005
Number of participants: 5
Phd Student: Villafafila Garcia, Ada (Intern)
Supervisor: Stenby, Erling Halfdan (Intern)
Main Supervisor: Thomsen, Kaj (Intern)
Examiner: Jensen, Jørgen Peter (Intern)
Kleinitz, Wolfram (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Integrated Process/Product Synthesis and Design Through a Reverse Modelling Approach

Department of Chemical and Biochemical Engineering
Period: 01/09/2002 → 07/03/2006
Number of participants: 5
Phd Student: d'Anterroches, Loïc (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Villadsen, John (Intern)
Kraslawski, Andrzej (Ekstern)
Pistikopoulos, Stratos (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Modeling, Design, Operability and Analysis of Reaction-Separation Systems
Department of Chemical and Biochemical Engineering
Period: 01/09/2002 → 07/03/2006
Number of participants: 5
Phd Student:
Ramirez Jimenez, Edgar (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Górak, Andrzej (Ekstern)
Perregaard, Jens (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Syntese og reformering af metanol
Department of Chemical and Biochemical Engineering
Period: 01/09/2002 → 24/01/2006
Number of participants: 6
Phd Student:
Andersen, Michael (Intern)
Supervisor:
Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Nerlov, Jesper (Intern)
Rupprechter, Günther (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Modelling of Pesticide Properties in Polymers and Pesticide Uptake in Plants Leafs
Department of Chemical and Biochemical Engineering
Period: 01/08/2002 → 07/03/2006
Number of participants: 5
Phd Student:
Muro Sunè, Nuria (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Abildskov, Jens (Ekstern)
Harper, Peter Mathias (Intern)
Heming, Alexander Mark (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Study of Alloy Catalysts for Production of Hydrogen
Department of Chemical and Biochemical Engineering
Period: 01/06/2002 → 22/09/2006
Number of participants: 5
Phd Student:
Boisen, Astrid (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Muhler, Martin (Ekstern)
Skoglundh, Bo Magnus (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Efficient and enviromentally friendly antifouling paints
Department of Chemical and Biochemical Engineering
Period: 01/05/2002 → 30/09/2005
Number of participants: 7
Phd Student:
Meseguer Yebra, Diego (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kil, Søren (Intern)
Examiner:
Villadsen, John (Intern)
Codolar, Santiago Arias (Ekstern)
Haslbeck, Elizabeth G. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Chemistry of Degradation of Cross-Linked Polymer
Department of Chemical and Biochemical Engineering
Period: 01/04/2002 → 15/07/2005
Number of participants: 6
Phd Student:
Mitra, Susanta (Intern)
Supervisor:
Almdal, Kristoffer (Intern)
Towards a Hydrogen-based Society

Experts stipulate that the world’s oil and gas resources will be emptied in less than a hundred years. Although the coal resources are significantly larger than those of oil and gas, coal cannot substitute oil and gas without severe environmental consequences. All major industrialized countries thus carry out intensive research to find clean and sustainable energy alternatives. Hydrogen is generally accepted as a possible future replacement of fossil fuels and it will play a crucial role as a new clean energy carrier. The vision of the so-called hydrogen society is to use renewable energy sources to produce hydrogen by simply dissociating water molecules. When the energy stored in hydrogen is converted into, e.g., electricity and heat in a fuel cell, water is formed again as the only by-product in a pollution-free and sustainable process. However, the technologies needed to realize this vision still require development and significant improvement before hydrogen presents a realistic alternative to the fossil fuel based energy system. To develop new schemes and improve existing technologies to produce and store hydrogen and to convert the energy in hydrogen to electricity, fundamental as well as more applied research must be performed. We propose the establishment of a large, interdisciplinary, inter-institutional research center with the main objective of carrying out research within the technologies associated with the hydrogen society. The center will comprise some of the most competent and internationally well-recognized research groups in Denmark within the proposed subjects. The balanced mix of fundamental research, carried out mainly by the university groups, and the more applied research, carried out by the industrial partners and groups at a national research center, ensures that all important aspects from basic science to commercialization of the hydrogen technologies are treated. The specific objectives of the proposed project are to - perform research and development on electrode catalysts for two different types of fuel cells - perform research and development on hydrogen storage materials such as metal hydrides - demonstrate small energy units based on the hydrogen technology - evaluate the implementation and implications of the hydrogen technology in the society

Department of Physics
Risø National Laboratory for Sustainable Energy
Department of Chemical and Biochemical Engineering
Center for Individual Nanoparticle Functionality
Center for Nanoteknologi
Aarhus University
IRD Fuel Cells A/S
Haldor Topsoe AS
Danfoss A/S

Period: 05/03/2002 → 31/12/2006
Number of participants: 6
Project ID: 20112
Project participant:
Besenbacher, Flemming (Ekstern)
Hammer, Bjørk (Ekstern)
Pedersen, Allan Scrøder (Ekstern)
Andersen, Steen Yde (Ekstern)
Clausen, Bjerne S. (Ekstern)

Project Manager, organisational:
Chorkendorff, Ib (Intern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Modelling, Simulation and Optimization of Anaerobic Biogas Processes

Department of Chemical and Biochemical Engineering
Period: 01/03/2002 → 30/04/2002
Number of participants: 2
Phd Student:
   Velusami, Balasubramanian (Intern)
Main Supervisor:
   Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

Kemisk Produktudvikling - Formulering og karakterisering af enzymgranulater

Department of Chemical and Biochemical Engineering
Period: 15/02/2002 → 07/11/2005
Number of participants: 7
Phd Student:
   Jørgensen, Kåre (Intern)
Supervisor:
   Bach, Pouli (Ekstern)
   Dam-Johansen, Kim (Intern)
Main Supervisor:
   Jensen, Anker Degn (Intern)
Examiner:
   Szabo, Peter (Ekstern)
   Hansen, Tomas T. (Ekstern)
   Lee, Geoffrey (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Oxidationsbeskyttelse af fiskeolieholdige produkter

Department of Chemical and Biochemical Engineering
Period: 01/01/2002 → 18/05/2007
Number of participants: 6
Phd Student:
   Bruni Lot, Mette (Intern)
Supervisor:
   Jacobsen, Charlotte (Intern)
Main Supervisor:
   Meyer, Anne S. (Intern)
Examiner:
   Jørgensen, Bo Munk (Intern)
   Andersen, Henrik Jørgen (Ekstern)
   Nilsson, Astrid (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD
Release of inorganic metal species, sulfur and chlorine during biomass combustion on a grate

Department of Chemical and Biochemical Engineering
Period: 01/01/2002 → 24/01/2006
Number of participants: 7
Phd Student:
vant Lith, Simone Cornelia (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Jensen, Peter Arendt (Intern)
Main Supervisor:
Giarborg, Peter (Intern)
Examiner:
Skrifvars, Bengt-Johan (Ekstern)
Pedersen, Lars Storm (Intern)
Unterberger, Sven (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Karakterisering af kemisk nedbrydning af polymerer

Department of Chemical and Biochemical Engineering
Period: 01/12/2001 → 25/06/2008
Number of participants: 6
Phd Student:
Kjellander, Carina Koch (Ekstern)
Supervisor:
Almdal, Kristoffer (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Szabo, Peter (Ekstern)
Gravesen, Per Otto Børresen (Ekstern)
Karlisson, Sigbritt (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Modelling for Predictive Control

Department of Chemical and Biochemical Engineering
Period: 01/11/2001 → 22/01/2007
Number of participants: 6
Phd Student:
Li, Hongwen (Ekstern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Abildskov, Jens (Ekstern)
Andersen, Henrik Weisberg (Ekstern)
Jacobsen, Elling W. (Ekstern)
**Transport Properties in Free Space and in a Porous Media**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2001 → 04/03/2005  
Number of participants: 5  
PhD Student:  
Medvedyev, Oleg (Ekstern)  
Main Supervisor:  
Shapiro, Alexander (Intern)  
Examiner:  
Hassager, Ole (Intern)  
Lindeloff, Niels (Intern)  
Wesselingh, Johannes (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Micro Structuring of Conducting Polymers**

Department of Chemical and Biochemical Engineering  
Period: 01/10/2001 → 10/01/2005  
Number of participants: 7  
PhD Student:  
Winther-Jensen, Bjørn (Intern)  
Supervisor:  
Menon, Aric Kumaran (Intern)  
West, Keld (Intern)  
Main Supervisor:  
Lyngaae-Jørgensen, Jørgen (Intern)  
Examiner:  
Hvilsted, Søren (Intern)  
Bechgaard, Klaus (Intern)  
Inganäs, Olle (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet  
Project: PhD

**Compositional Streamline Simulation**

Department of Chemical and Biochemical Engineering  
Period: 01/09/2001 → 28/01/2005  
Number of participants: 7  
PhD Student:  
Berenblyum, Roman (Ekstern)  
Supervisor:  
Michelsen, Michael Locht (Intern)  
Shapiro, Alexander (Intern)  
Main Supervisor:  
Stenby, Erling Halfdan (Intern)  
Examiner:  
Foged, Niels Tækker (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: PhD
Bedrikovetsky, Pavel (Ekstern)
Jakupsstovu, Sigurd (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden sektorministeriel finans
Project: PhD

Dielektriske elastomer aktuatorer
Department of Chemical and Biochemical Engineering
Period: 01/08/2001 → 23/08/2004
Number of participants: 5
Phd Student:
Skov, Anne Ladegaard (Intern)
Supervisor:
Sommer-Larsen, Peter (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Keunings, Roland (Ekstern)
Ndoni, Sokol (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Modellering af ionbytningsprocesser med koncentrerede elektrolytopløsninger
Department of Chemical and Biochemical Engineering
Period: 01/08/2001 → 04/07/2005
Number of participants: 5
Phd Student:
Christensen, Søren Gregers (Intern)
Supervisor:
Mollerup, Jørgen (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Ivar Andersen, Simon (Intern)
Hansen, Ernst (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Tilstopning af katalysatormonolitter som anvendes i selektiv katalytisk reduktion af NOx i støvbelastede gastrømme
Department of Chemical and Biochemical Engineering
Period: 01/08/2001 → 30/09/2002
Number of participants: 3
Phd Student:
Hansen, Carsten (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Transport Coefficients in Hydrocarbon Mixtures under Microgravity Conditions

Department of Chemical and Biochemical Engineering
Period: 01/08/2001 → 18/03/2005
Number of participants: 6
PhD Student: Gonzales Bagnoli, Mariana G. (Intern)
Supervisor: Stenby, Erling Halfdan (Intern)
Main Supervisor: Shapiro, Alexander (Intern)
Examiner: Mollerup, Jørgen (Intern), Knudsen, Kim (Intern), Montel, François (Ekstern)

Hybrid Modeling for Bioreactor Performance

Department of Chemical and Biochemical Engineering
Period: 15/05/2001 → ...
Number of participants: 7
PhD Student: Thaysen, Mads (Intern)
Supervisor: Petersen, Jørgen (Ekstern), Steffensen, Erik (Ekstern)
Main Supervisor: Jørgensen, Sten Bay (Intern)
Examiner: Villadsen, John (Intern), Gram, Jens (Ekstern), Stockar, Urs von (Ekstern)

Emissioner fra forbrænding af biomasse

Department of Chemical and Biochemical Engineering
Period: 01/04/2001 → 10/01/2005
Number of participants: 7
PhD Student: Knudsen, Jacob Nygaard (Intern)
Supervisor: Jensen, Peter Arendt (Intern)
Main Supervisor: Lin, Weigang (Intern)
Examiner: Dam-Johansen, Kim (Intern)
Livbjerg, Hans (Intern)
Hupa, Mikko (Ekstern)
Pedersen, Lars Storm (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Nordisk finansiering
Project: PhD

**Computer Aided Development and Optimization of Chromatographic Separators**
Department of Chemical and Biochemical Engineering
Period: 01/03/2001 → 10/11/2004
Number of participants: 6
Phd Student:
Frederiksen, Søren Søndergaard (Intern)
Supervisor:
Hansen, Ernst (Intern)
Michelsen, Michael Locht (Intern)
Main Supervisor:
Mollerup, Jørgen (Intern)
Examiner:
Villadsen, John (Intern)
Staby, Arne (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**A Group Contribution Cubic Equation of State for Paints**
Department of Chemical and Biochemical Engineering
Period: 01/02/2001 → 22/04/2004
Number of participants: 6
Phd Student:
Kouskoumvekaki, Eirini (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Mollerup, Jørgen (Intern)
Dahl, Søren (Ekstern)
Voutsas, Epaminondas C. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

**Petroleumsresiners Kemiske Egenskaber og Vekselvirkninger med Asphaltener i Olie**
Department of Chemical and Biochemical Engineering
Period: 01/02/2001 → 12/05/2004
Number of participants: 4
Phd Student:
Garcia, Daniel Merino (Intern)
Main Supervisor:
Ivar Andersen, Simon (Intern)
Examiner:
Thomsen, Kaj (Intern)
Sjöblom, Johan E. G. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

Reaction Pathway Analysis
Department of Chemical and Biochemical Engineering
Period: 01/02/2001 → 01/05/2007
Number of participants: 6
Phd Student:
Hansen, Morten Skov (Intern)
Supervisor:
Villadsen, John (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Olsson, Lisbeth (Intern)
Diers, Ivan Verner (Ekstern)
Sonnleitner, Bernhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden sektorministeriel finans
Project: PhD

Mætningsfordeling og petrofysiske egenskaber i lav-permable Nordø kalkreservoirer
Department of Chemical and Biochemical Engineering
Period: 16/11/2000 → 09/12/2005
Number of participants: 2
Phd Student:
Nielsen, Carsten Møller (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
Project: PhD

Dissolution and Adsorption of Light Hydrocarbons in Drilling Muds, Prediction of the Nature of a REsevoir Fluid Based on Gas Shows
Department of Chemical and Biochemical Engineering
Period: 01/10/2000 → 14/07/2006
Number of participants: 6
Phd Student:
Lige, Xavier Christophe (Intern)
Supervisor:
Shapiro, Alexander (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Fabricius, Ida Lykke (Intern)
Marnat, Serge (Ekstern)
Øbro, Hans (Ekstern)
**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samarbejdssavlefinans  
Project: PhD

**Cyklon forvarmerdesign med henblik på emissionsbegrænsning i cementindustrien**  
Department of Chemical and Biochemical Engineering  
Number of participants: 7  
Phd Student:  
Hansen, Jens Peter (Intern)  
Supervisor:  
Jensen, Lars Skaarup (Intern)  
Wedel, Stig (Ekstern)  
Main Supervisor:  
Dam-Johansen, Kim (Intern)  
Examiner:  
Johnsson, Jan Erik (Intern)  
Hansen, Peter F. Binderup (Ekstern)  
Hupa, Mikko (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Erhvervsforskerordningen  
Project: PhD

**Fremstilling og test af katalytiske materialer**  
Department of Chemical and Biochemical Engineering  
Period: 01/09/2000 → 10/01/2005  
Number of participants: 6  
Phd Student:  
Mosleh, Majid (Ekstern)  
Supervisor:  
Johansson, Tue (Intern)  
Main Supervisor:  
Livbjerg, Hans (Intern)  
Examiner:  
Jonsson, Gunnar Eigil (Intern)  
Christensen, Kurt Agerbæk (Ekstern)  
Christiansen, Niels (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD

**Structures and properties of polymer blends and alloys. Influence of Diblock Copolymers.**  
Department of Chemical and Biochemical Engineering  
Number of participants: 5  
Phd Student:  
Chuai, Chengzhi (Intern)  
Supervisor:  
Almdal, Kristoffer (Intern)  
Main Supervisor:  
Lyngaae-Jørgensen, Jørgen (Intern)  
Examiner:  
Kjær, Erik Michael (Intern)
Pedersen, Walther Batsberg (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

**Intelligente Klæbere**
Department of Chemical and Biochemical Engineering
Period: 01/08/2000 → 13/08/2004
Number of participants: 8
Phd Student:
Hansen, Kristoffer Karsten (Intern)
Supervisor:
Almdal, Kristoffer (Intern)
Christensen, Søren Flygenring (Intern)
Samuelsen, Peter (Intern)
Main Supervisor:
Hvilsted, Søren (Intern)
Examiner:
Lyngaae-Jørgensen, Jørgen (Intern)
Gedde, Ulf W. (Ekstern)
Rehnberg, Nicola (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

**Optimal and Reproducible Operation of Batch Processes**
Department of Chemical and Biochemical Engineering
Period: 01/08/2000 → 08/07/2005
Number of participants: 5
Phd Student:
Bonné, Dennis (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Poulsen, Niels Kjølstad (Intern)
Andersen, Henrik Weisberg (Ekstern)
Bonvin, Dominique (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden sektorministeriel finans
Project: PhD

**Integration of synthesis, design and control of batch operations for product design**
Department of Chemical and Biochemical Engineering
Period: 01/06/2000 → 07/03/2006
Number of participants: 5
Phd Student:
Papaoikonomou, Eirini (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Membrane Modification

Department of Chemical and Biochemical Engineering
Period: 15/05/2000 → 19/03/2004
Number of participants: 7
PhD Student:
Kæselev, Bozena Alicja (Intern)
Supervisor:
Belfort, Georges (Ekstern)
Olsen, Ole Jentoft (Ekstern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Hvilsted, Søren (Intern)
Aptel, Philippe (Ekstern)
Kristensen, Steen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden sektorministeriel finans
Project: PhD

Phase behavior and transport processes in porous media

Department of Chemical and Biochemical Engineering
Period: 01/04/2000 → 28/02/2001
Number of participants: 2
PhD Student:
Madsen, Jesper (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Prediction of the solubility of polymers in aqueous and mixed solvents

Department of Chemical and Biochemical Engineering
Number of participants: 6
PhD Student:
Lindvig, Thomas (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Mollerup, Jørgen (Intern)
Elbro, Helle Simon (Ekstern)
Sadowski, Gabriele (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**A structural study of block copolymers under deformation**

Department of Management Engineering
Department of Chemical and Biochemical Engineering
Forskningscenter Risø
Period: 01/02/2000 → 01/01/2003
Number of participants: 4
Project participant:
Kjær, Erik Michael (Intern)
Eskimergen, Rüya (Intern)
Mortensen, Kell (Intern)
Vigild, Martin Etchells (Intern)

**Financing sources**
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 1,077,000.00 Danish Kroner
Project: Design, dynamik og regulering af integrerede processer

Department of Chemical and Biochemical Engineering
Period: 01/02/2000 → 31/03/2002
Number of participants: 2
Phd Student:
Skotte, René (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

**Karakterisering af polymersmelter i forlængelse**

Department of Chemical and Biochemical Engineering
Period: 01/02/2000 → 24/10/2003
Number of participants: 6
Phd Student:
Bach, Anders (Ekstern)
Supervisor:
Almdal, Kristoffer (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Lyngaae-Jørgensen, Jørgen (Intern)
McLeish, Thomas (Ekstern)
Meissner, Joachim (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Nanosensorer for orientering og mekanisk spænding i polymermaterialer

Department of Chemical and Biochemical Engineering
Period: 01/02/2000 → 27/05/2003
Number of participants: 7
PhD Student: Spanggaard, Holger (Intern)
Supervisor: Almdal, Kristoffer (Intern)
Jørgensen, Mikkel (Intern)
Main Supervisor: Kops, Jørgen (Intern)
Examiner: Hassager, Ole (Intern)
Jannasch, Patric (Ekstern)
Ogilby, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Project: PhD

Modellering, ikke-lineær Dynamik og irreversibel termodynamik (MIDIT)


Department of Informatics and Mathematical Modeling
Department of Mathematics
Department of Physics
Administration
Department of Chemistry
Department of Energy Engineering
Period: 01/01/2000 → 31/12/2002
Number of participants: 1
Project Manager, organisational: Christiansen, Peter Leth (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 360,000.00 Danish Kroner
Project
**Phase behavior of Aqueous of Surfactant Solution**

Department of Chemical and Biochemical Engineering  
Period: 01/01/2000 → 26/02/2004  
Number of participants: 6

Phd Student:  
Cheng, Hongyuan (Intern)  
Supervisor:  
Kontogeorgis, Georgios (Intern)  
Main Supervisor:  
Stenby, Erling Halfdan (Intern)  
Examiner:  
Ivar Andersen, Simon (Intern)  
Birdi, Kulbir S. (Ekstern)  
Maurer, Gerd (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Centerfinansieret  
Project: PhD

**CEVI method development**  
The project aimed at developing operational methods for savings and reuse of water and waterborne energy and chemicals in industrial wet processing. Methods include simple pinch analyses for targeting water savings and -reuse as well as methods for system design of water reuse systems. Moreover procedures for identifying options for process optimisation were developed including savings of water, energy, and chemicals. Finally, the feasibility of separation technologies such as membranefiltration and evaporation was revealed through laboratory and pilot scale test procedures. Solutions of large savings and short economic pay-back periods were chosen and successfully implemented in full scale.
**Financing sources**
Source: Forsk. Andre statslige danske i øvrigt  
Name of research programme: Forsk. Andre statslige danske i øvrigt  
Amount: 1,500,000.00 Danish Kroner  
Project

**Fouling and scaling in membrane processes: Mechanisms and how to control these phenomena**
Department of Chemical and Biochemical Engineering  
Period: 15/11/1999 → 12/05/2004  
Number of participants: 4  
Phd Student:  
Lipnizki, Jens (Intern)  
Main Supervisor:  
Jonsson, Gunnar Eigil (Intern)  
Examiner:  
Wenzel, Henrik (Intern)  
Kristensen, Steen (Ekstern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: Centerfinansieret  
Project: PhD

**Modellering af soddannelse**
Department of Chemical and Biochemical Engineering  
Period: 01/11/1999 → 05/09/2003  
Number of participants: 9  
Phd Student:  
Skjøth-Rasmussen, Martin Skov (Intern)  
Supervisor:  
Jensen, Anker Degn (Intern)  
Johannessen, Tue (Intern)  
Livbjerg, Hans (Intern)  
Østberg, Martin (Intern)  
Main Supervisor:  
Glarborg, Peter (Intern)  
Examiner:  
Wedel, Stig (Ekstern)  
Lindstedt, Peter (Ekstern)  
Rasmussen, Niels Bjarne Kampp (Ekstern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: Erhvervsforskerordningen  
Project: PhD

**Modellering af gipsproducerede røggasafsvolingsanlæg**
Department of Chemical and Biochemical Engineering  
Period: 01/10/1999 → 13/12/2005  
Number of participants: 9  
Phd Student:  
Nygaard, Helle Gottschalk (Intern)  
Supervisor:  
Dam-Johansen, Kim (Intern)  
Fogh, Folmer (Ekstern)  
Jensen, Jørgen Nørklit (Ekstern)  
Kiil, Søren (Intern)
Main Supervisor:
Johnsson, Jan Erik (Intern)
Examiner:
Wedel, Stig (Ekstern)
Jensen, Flemming (Ekstern)
Karlsson, Hans T. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Thermodynamic insights based integration of process synthesis, design and control
Department of Chemical and Biochemical Engineering
Period: 01/10/1999 → 28/02/2003
Number of participants: 5
Phd Student:
Bek-Pedersen, Erik (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Górak, Andrzej (Ekstern)
Sørensen, Esben Lauge (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Måling og modellering af væske-væske-gas ligevægte ved høje tryk
Department of Chemical and Biochemical Engineering
Period: 01/08/1999 → 25/04/2003
Number of participants: 6
Phd Student:
Laursen, Torben (Intern)
Supervisor:
Rasmussen, Peter (Intern)
Main Supervisor:
Ivar Andersen, Simon (Intern)
Examiner:
Mollerup, Jørgen (Intern)
Artt, Wolfgang (Ekstern)
Maurer, Gerd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Nonlinear identification and optimal control of fed-batch processes
Department of Chemical and Biochemical Engineering
Period: 01/08/1999 → 24/03/2003
Number of participants: 6
Phd Student:
Kristensen, Niels Rode (Intern)
Supervisor:
Madsen, Henrik (Intern)
Synthesis of Amphiphilic Block Copolymers by ATRP in Aqueous Systems

New techniques for controlled radical polymerization are applied for formation of complex polymer systems, particularly amphiphilic block copolymers to obtain new molecular design of materials for potential new applications.

Department of Chemical and Biochemical Engineering
Period: 01/07/1999 → 30/06/2002
Number of participants: 1

Project Manager, organisational: Kops, Jørgen (Intern)

Alternative Methods for Energy-Efficient Material Separations

Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 21/12/2003
Number of participants: 6

PhD Student: Eden, Mario Richard (Intern)
Supervisor: Gani, Rafiqul (Intern)
Main Supervisor: Jørgensen, Sten Bay (Intern)
Examiner: Kiil, Søren (Intern)
Cordiner, Joan (Ekstern)
Kraslawski, Andrzej (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt CAMP
Project: PhD

Chromatographic Separation of Whey Proteins
Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 27/05/2003
Number of participants: 4
Phd Student:
Pedersen, Linda (Intern)
Main Supervisor:
Mollerup, Jørgen (Intern)
Examiner:
Ivar Andersen, Simon (Intern)
Müller, Egbert (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Global CAPE-OPEN
EU-Funded project
Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 31/12/2001
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner
Project

Grænseflader i komposite elektroder i fastoxid - brændseelsceller/elektrolysatorer
Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 09/09/2002
Number of participants: 8
Phd Student:
Hansen, Karin Vels (Intern)
Supervisor:
Bilde-Sørensen, Jørgen (Intern)
Chorkendorff, Ib (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Jacobsen, Torben (Ekstern)
Hansen, Poul Lenvig (Ekstern)
Stimming, Ulrich (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Nordisk Finansiering-SU
Project: PhD
Optimisation Techniques for Process Synthesis, Design and control
Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 31/03/2001
Number of participants: 2
Phd Student:
Henriksen, Jens Peter (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt EU-finansieret
Project: PhD

Fasefordeling af produktionskemikalier
Department of Chemical and Biochemical Engineering
Period: 01/05/1999 → 21/02/2003
Number of participants: 6
Phd Student:
Derawi, Samer (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Ivar Andersen, Simon (Intern)
Economou, Ioannis (Intern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt CAMP
Project: PhD

Development of a Mathematical Model for Simulation, Design and Control of a Cupola Furnace
Department of Chemical and Biochemical Engineering
Period: 01/04/1999 → ...
Number of participants: 9
Phd Student:
Leth-Miller, Rasmus (Intern)
Supervisor:
Glarborg, Peter (Intern)
Hansen, Peter F. Binderup (Ekstern)
Jensen, Leif Møller (Ekstern)
Jensen, Anker Degn (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Livbjerg, Hans (Intern)
Bhatia, Vinay K. (Ekstern)
Sarofim, Adel F. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD
**PRIORITIES - Improved Oil Recovery and Productivity from Lower Cretaceous Carbonates**

Joint project between IVC-SEP and the Geological Survey of Denmark, Sponsored by the EFP programs EFP-97 and EFP-99.

Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

Period: 01/03/1999 → 31/12/2002

Number of participants: 1

Project Manager, organisational:

Jørgensen, Marianne (Intern)

Project

**Computer Aided Process/Phenomena Modelling Based on Data**

Department of Chemical and Biochemical Engineering

Period: 01/02/1999 → 15/03/2001

Number of participants: 2

Phd Student:

Nielsen, Thomas Lund (Intern)

Main Supervisor:

Gani, Rafiqul (Intern)

**Financing sources**

Source: Internal funding (public)

Name of research programme: DTU-lønnet stipendie

Project: PhD

**Diffusion in liners in offshore flexible pipes**

Flexible high pressure pipes are increasingly used in marine environments for the transportation of well fluids. A flexible pipe consists typically of an inner and outer polymer tube (inner lining and outer sheath), with a number of helically wound steel armour profiles in between. The purpose of the inner lining is to provide the pipe with a leak tight barrier against the transported fluids whereas the outer sheath protects the armour wires from the external environment, e.g. the sea water. A supporting metallic carcass may be applied internally in the pipe bore to increase the collapse strength of the inner lining.

The objective of this project is to establish a reliable method for calculating the resulting concentrations of methane, carbon dioxide and hydrogen sulphide in the annulus of flexible high pressure pipes when subjected to varying operational conditions.

Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

NKT Research & Innovation A/S

NKT Flexibles A/S

Period: 01/01/1999 → 31/12/2001

Number of participants: 5

Project participant:

Hassager, Ole (Intern)

Kristensen, Susanne Brogaard (Intern)

Marcher, Bjørn (Ekstern)

Nielsen, Niels Rishøj (Ekstern)

Project Manager, organisational:

Szabo, Peter (Intern)

**Financing sources**

Source: Unknown

Name of research programme: Ukendt

Amount: 1,200,000.00 Danish Kroner

Project
Engeneering model of natural gas reburning

Department of Chemical and Biochemical Engineering
Period: 01/01/1999 → …
Number of participants: 7
Phd Student: Schmidt, Lone Mønsted (Intern)
Supervisor: Jensen, Anker Degn (Intern)
Rasmussen, Niels Bjarne Kampp (Ekstern)
Main Supervisor: Glarborg, Peter (Intern)
Examiner: Johnsson, Jan Erik (Intern)
Hupa, Mikko (Ekstern)
Østberg, Martin (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Engineering model of natural gas reburning

NOx emissions from fossil fuel and biomass fired combustors are causing concern due to harmful environmental effects such as photochemical smog and acid rain. Reburning, which is a process to limit the emission of NOx by using natural gas as reducing agent, has been found to be an effective process. Current design of gas injection systems however, rely on models for the flow and not the combined effect of flow and chemistry taking place in the jet. The current project aims at developing an engineering model that provides a detailed description of the reburn chemistry in combination with the flow in the jet-mixing system.

Department of Chemical and Biochemical Engineering

Danish Gas Technology Centre A/S
Period: 01/01/1999 → 31/12/2000
Number of participants: 2
Project participant: Glarborg, Peter (Intern)
Project Manager, organisational: Jensen, Anker Degn (Intern)
Project

Termodynamisk model for korrelation af opløseligheden af aminosyrer i vandige opløsninger

Department of Chemical and Biochemical Engineering
Period: 01/10/1998 → 14/03/2002
Number of participants: 5
Phd Student: Breil, Martin Peter (Intern)
Main Supervisor: Mollerup, Jørgen (Intern)
Examiner: Kontogeorgis, Georgios (Intern)
Hansen, Ernst (Intern)
Maurer, Gerd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt CAMP
Project: PhD

Hygienic Design of Food Processing Machinery

Hygienic design of machinery for production of foods is essential when producing high quality and safe foods. The project is concerned with optimisation of equipment design by studying the flow patterns inside closed equipment. The flow
conditions will be related to deposit of fouling material and the subsequent removal of this. Computational Fluid Mechanics (CFD) is used to describe the flow and design a method for optimisation of equipment design. A correlation between wall shear stresses needed for removal of soil under well-defined flow conditions in a Radial Flow Cell (RFC) and CFD simulations is determined. A CFD model describing the flow pattern in a plug valve is in the progress of being modified to describe similar removal of soil in the valve. Preliminary results show that the wall shear stress is not the sole flow parameter, which influences cleaning. Flow phenomena like locally large turbulence are expected to contribute significantly to the mechanical cleaning effect. The project is a part of a larger centre contract from Erhvervsfremme Styrelsen.

Department of Biotechnology
Department of Chemical and Biochemical Engineering

Alfa Laval Flow
Period: 01/09/1998 → 31/12/2001
Number of participants: 4
Project participants:
Jensen, Bo Boye Busk (Intern)
Adler-Nissen, Jens (Intern)
Szabo, Peter (Intern)
Project Manager, organisational:
Fris, Alan (Intern)

Kinetic theory of linear and branched polymers in shear-free deformations
Department of Chemical and Biochemical Engineering
Period: 01/09/1998 → 15/01/2002
Number of participants: 6
Phd Student:
Neergaard, Jesper (Intern)
Supervisor:
Schieber, Jay (Ekstern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Szabo, Peter (Ekstern)
Hulsen, M. A. (Ekstern)
Keunings, Roland (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Storage strategies for historical plastics
Department of Chemical and Biochemical Engineering
Period: 01/09/1998 → 14/12/2001
Number of participants: 4
Phd Student:
Shashoua, Yvonne (Intern)
Main Supervisor:
Kops, Jørgen (Intern)
Examiner:
Hvilsted, Søren (Intern)
Holmström, Karl Arne (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD
**Aerosol routes to catalytic materials**
Catalytic materials are synthesized via flame generated nano-particles and by other aerosol-based methods. The catalysts are tested by various chemical and physical methods.

Department of Chemical and Biochemical Engineering
Department of Manufacturing Engineering
Interdisciplinary Center for Catalysis

**Period**: 01/08/1998 → …
**Number of participants**: 5
**Project participant**: 
Wedel, Stig (Ekstern)
Johannessen, Tue (Intern)
Jensen, Joakim Reimer (Intern)
Beckerslev, Bente (Intern)

**Project Manager, organisational**: 
Livbjerg, Hans (Intern)

**Financing sources**
**Source**: Unknown
**Name of research programme**: Ukendt
**Amount**: 3,000,000.00 Danish Kroner

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**Computational Fluid-Particle Dynamics**
Computational Fluid dynamics (CFD) is combined with models for particle dynamics in order to simulate nano-particle formation in High-Temperature processes (e.g. flames)

Department of Chemical and Biochemical Engineering

**Period**: 01/08/1998 → …
**Number of participants**: 2
**Project participant**: 
Livbjerg, Hans (Intern)

**Project Manager, organisational**: 
Johannessen, Tue (Intern)

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**Fremstilling af katalytiske materialer ved Aerosolmetoder**

Department of Chemical and Biochemical Engineering

**Period**: 01/08/1998 → 07/03/2002
**Number of participants**: 6
**Phd Student**: 
Jensen, Joakim Reimer (Intern)

**Supervisor**: 
Wedel, Stig (Ekstern)

**Main Supervisor**: 
Livbjerg, Hans (Intern)

**Examiner**: 
Fehrmann, Rasmus (Intern)
Nielsen, Poul Erik Højlund (Ekstern)
Pratsinis, Sotiris E. (Ekstern)

**Financing sources**
**Source**: Internal funding (public)
**Name of research programme**: DTU-lønnet stipendie

**Project**: PhD
Kompositionel reservoirsimulering af gas injektionsprocesser

Department of Chemical and Biochemical Engineering
Period: 01/08/1998 → 28/02/2003
Number of participants: 5
Phd Student: Jakupsstovu, Sigurd (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)
Examiner: Shapiro, Alexander (Intern)
Jansson, John (Ekstern)
Olsen, Henrik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Kandidatstipendium ansat på DT
Project: PhD

Beregningsmodeller til optimering af sukkerkrystalisation

Department of Chemical and Biochemical Engineering
Period: 01/05/1998 → 11/11/2001
Number of participants: 5
Phd Student: Rasmussen, Angelique Grønborg (Intern)
Main Supervisor: Rasmussen, Peter (Intern)
Examiner: Mollerup, Jørgen (Intern)
Azevedo, Sebastiao Feyo de (Ekstern)
Jacobsen, Carsten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Kulbrinters egenskaber ved høje tryk og temperaturer

Department of Chemical and Biochemical Engineering
Number of participants: 5
Phd Student: Zeberg-Mikkelsen, Claus Kjær (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)
Examiner: Fernández, Josefa (Ekstern)
Knudsen, Kim (Intern)
Thomsen, Kaj (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt EU-finansieret
Project: PhD

MENUSIM Web Network.
The objectives of the full MENUSIM network were firstly to set up an efficient platform for exchange and discussion between numerical modelling and measurement specialists in the field of polymer materials processing, secondly to favour a better orientation of R&D activities with respect to unsolved practical problems, and thirdly to promote the transfer of knowledge from university research laboratories to industry. The chosen platform was a Web network fed through a
dedicated server that gives free access to MENUSIM forum but preserves the filtered and synthesized monthly information to subscribers. http://www.meca.ucl.ac.be/memawww/menusim

Department of Chemical and Biochemical Engineering

Universite Pierre et Marie Curie

DIKautschuck

Hutchinson

JL Consulting

Pirelli Pneumatici S.p.A.

SOLVAY S.a.

SPEC Process Services

Universite Catholique de Louvain

University of Freiburg

Loughborough University

University of Minho

VTT - Technical Research Centre of Finland

ARTTIC

Period: 01/04/1998 → 30/11/1999

Number of participants: 15

Project participant:

Hassager, Ole (Intern)

Leblanc, Jean Leopold (Ekstern)

Uphus, Reinhard (Ekstern)

Karam, Simon (Ekstern)

Doumont, Jean-Luc (Ekstern)

Nichitti, Dario (Ekstern)

Dehennau, Mr. Claude (Ekstern)

Mitsoulis, Evan (Ekstern)

Legat, Vincent (Ekstern)

Friedrich, Christian (Ekstern)

Freakley, Philip K. (Ekstern)

Covas, Jose A. (Ekstern)

Valta, Kyosti (Ekstern)

Lagarde, Pierre (Ekstern)

Project Manager, organisational:

Szabo, Peter (Intern)

Financing sources

Source: Unknown

Name of research programme: Ukendt

Amount: 70,000.00 Danish Kroner

Project

Modellering af kulbrinteblandingers faseopførsel ved høje tryk og temperaturer

Department of Chemical and Biochemical Engineering


Number of participants: 5

Phd Student:

Halldórsson, Snorri (Intern)

Main Supervisor:

Stenby, Erling Halfdan (Intern)

Examiner:
Deactivation of catalysts for selective catalytic reduction of NO
Selective catalytic reduction (SCR) of NO by ammonia is the most common secondary measure to limit the emission of NO from combustion processes. This technology is well proven on coal fired power plants. However, on biomass fired boilers or coal-biomass co-fired boilers, the SCR catalysts have been found to deactivate much faster, probably related to the higher content of potassium in the straw compared to coal. The aim of this project is to investigate the cause of this deactivation and if possible, suggest a cure. The project involves experiments in full-scale, pilot-scale and in the laboratory, detailed characterization of the deactivated catalysts and test of methods to regenerate the catalysts.

Department of Chemical and Biochemical Engineering
Period: 01/02/1998 → 31/12/2001
Number of participants: 1
Project Manager, organisational:
Jensen, Anker Degn (Intern)
Project

HYSEP
EU-Funded project

Department of Chemical and Biochemical Engineering
Period: 01/02/1998 → 01/02/2001
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 800,000.00 Danish Kroner
Project
Integrated Simulation System with thermodynamic insight

Department of Chemical and Biochemical Engineering
Period: 01/02/1998 → 01/11/2000
Number of participants: 3
Phd Student: Russel, Boris Mariboe (Intern)
Supervisor: Jørgensen, Sten Bay (Intern)
Main Supervisor: Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Project: PhD

Product Recovery for Spray Dryers
In most drying technologies either product recovery or gas cleaning are important unit operations. The dry product is suspended in the drying gas, and the particles have to be separated from the gas before further processing. This may be done by cyclones or filters or a combination thereof. The present project focuses on the filtration step. The aim of the project is to be able to perform accurate design of the filter system and required filter area for a given powder. The project consists of the following parts: 1) Development of laboratory methods to measure and predict the pressure loss over a filter cake as a function of velocity, temperature, humidity, powder load etc. 2) Compare the laboratory results with results from full scale 2) Perform calculations by the use of Computational Fluid Dynamics (CFD) of the gas and particle flow within industrial size filter housing including the deposition of particles on the filter bags.

Department of Chemical and Biochemical Engineering
GEA Niro A/S
Period: 01/02/1998 → 31/12/2000
Number of participants: 1
Project Manager, organisational: Jensen, Anker Degn (Intern)

Project recovery from spray dryers

Department of Chemical and Biochemical Engineering
Period: 01/02/1998 → 20/04/2001
Number of participants: 6
Phd Student: Frey, Marcus (Intern)
Supervisor: Dam-Johansen, Kim (Intern)
Main Supervisor: Jensen, Anker Degn (Intern)
Examiner: Johnsson, Jan Erik (Intern)
Seville, Jonathan P. K. (Ekstern)
Lind, Leif (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Adsorptive and Chromatographic Behaviour of Proteins (D.1)
Measurement and modelling of: Separation of whey proteins, including measurement and modelling of: - Isotherms and retention factors - Gradient elution - Frontal analysis - Mass transfer

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 4
Project participant:

Borgbjerg, Ulrik (Intern)
Bisgaard-Frantzen, Hans (Intern)
Hansen, Ernst (Intern)

Project Manager, organisational:

Mollerup, Jørgen (Intern)

Changes in Product Stability during Hydrocracking (B.2)
Measurements of stability lines and parameters for evaluation of hydrotreatment processes. A M.Sc. Project is initiated in this area to further explore the use of flocculation titration.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 3
Project participant:

Dang, Tran Thuong (Intern)
Tecle, Zacarias (Intern)

Project Manager, organisational:

Ivar Andersen, Simon (Intern)

Computation of Phase Equilibria for Electrolyte Solutions (A.7)
- To further extend the applicability of the Extended UNIQUAC model to calculate gas solubility in and salt precipitation from a multi-ion aqueous solution at high pressure and temperature. - The solubility of SO2 and O2 in aqueous electrolyte solutions will be examined.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 2
Project participant:

Thomsen, Kaj (Intern)

Project Manager, organisational:

Rasmussen, Peter (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 76,400.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 76,400.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 76,400.00 Danish Kroner

Estimation of Properties based on the Group Contribution Approach (A.9)
To develop a new version of UNIFAC with second-order group contribution.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 2
Project participant:

Abildskov, Jens (Ekstern)

Project Manager, organisational:

Rasmussen, Peter (Intern)
Experiments with Electrolyte Solutions (A.2)
To measure salt solubility in steam.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Rasmussen, Peter (Intern)

Field measurements of combustion aerosols
The flue gas particles of power boilers are characterized with respect to 1) Penetration through electrostatic precipitators
2) Formation, behaviour, penetration, chemical composition and trace element content of PM2.5 3) Emission of particles
and contained elements.

Department of Chemical and Biochemical Engineering
Department of Manufacturing Engineering
RISØ
FLS Miljø A/S
Elkraft A.m.b.A.
Elsamprojekt A/S
Period: 01/01/1998 → ...
Number of participants: 3
Project participant:
Nielsen, Morten Thellefsen (Intern)
Beckerslev, Bente (Intern)
Project Manager, organisational:
Livbjerg, Hans (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,500,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 4,500,000.00 Danish Kroner

Fundamental aspects of asphaltenes in solutions (B.1)
Investigation of colloidal properties of fractionated asphaltenes

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 5
Project participant:
Pedersen, Carsten (Intern)
Dang, Tran Thuong (Intern)
Petersen, Karin (Intern)
Tecle, Zacarias (Intern)
Project Manager, organisational:
Ivar Andersen, Simon (Intern)

Gas Hydrate Formation (C.4)
To obtain a better understanding of the nucleation and growth of gas hydrates

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Rasmussen, Peter (Intern)

**IVC-SEP Program Package (B.1)**
During the last decades, a great number of programs has been developed for the analysis of phase equilibria and the design of separation processes of simple and complex mixtures. The IVC-SEP has contributed with many of these programs which are used in this and other institutions around the world. In order to continue with this contribution, we are working on two main objectives: the development of a new user interface and the creation of a standard subroutine library. The user interface will integrate the majority of programs and databases within the IVC-SEP in a user friendly framework. The library of standard subroutines will simplify the reuse of our programs by internal and external users.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1999
Number of participants: 1
Project Manager, organisational:
Pretel, Eduardo (Intern)

**Liquid-Liquid Equilibrium (LLE) Measurements (A.3)**
- To measure phase split in polymer solutions.
- To make LLE measurements on various propionates/acetic acid/water systems.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 2
Project participant:
Persson, Ole Hilding (Intern)
Project Manager, organisational:
Rasmussen, Peter (Intern)

**Measurement of Phase Equilibria and Transport Properties (C.2)**
PVT studies on petroleum reservoir fluids in the fibre optic mini PVT cell and the Mercury free ROP set-up. True boiling point (TBP) distillation of dead crude oils and gas condensates. Assessment of purity of TBP fractions by gas chromatographic (GC) analysis. Measurement of the viscosity of TBP cuts, dead crude oils, and gas condensates using the Anton-Paar microviscometer.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 4
Project participant:
Dandekar, Abhijit (Intern)
Dang, Tran Thuong (Intern)
Tecle, Zacarias (Intern)
Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

**Measurements of Various Thermophysical Properties (A.4)**
The project is temporarily suspended.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Rasmussen, Peter (Intern)
Modelling and Optimization of Sugar Crystallization (A.10)
To examine the influence of nonsugars (amino acids, salts, monosaccharides, proteins etc) on the crystallization of sugar. The idea is to find some characteristic impurity substances. Experiments in the laboratory are to be carried out to reveal important questions about the crystallization kinetics with model impurities.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Rasmussen, Peter (Intern)

Modelling of Phase Equilibria and Transport Properties (C.1)
Modelling of the phase behavior of reservoir fluids within a porous medium and during injection of gases.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 5
Project participant:
Michelsen, Michael Locht (Intern)
Shapiro, Alexander (Intern)
Dandekar, Abhijit (Intern)
Jessen, Kristian (Intern)
Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

Modelling of Phase Equilibria of Polymer Solutions (A.6)
To continue work on microphase separation in diblock copolymers.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 2
Project participant:
Pretel, Eduardo (Intern)
Project Manager, organisational:
Rasmussen, Peter (Intern)

Models for Transport Properties (A.8)
The project is currently inactive

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Rasmussen, Peter (Intern)

Phase Behavior of Asphaltene Containing Reservoir Fluids (C.5)
Developed procedures for correlation and prediction of the onset of asphaltene precipitation.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 5
Project participant:
Pedersen, Carsten (Intern)
Dang, Tran Thuong (Intern)
Lindeloff, Niels (Intern)
Tecle, Zacarias (Intern)
Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

**Phase Equilibria Including an Aqueous Phase (C.3)**
Prediction of phase equilibria of brine - oil systems containing production chemicals. An investigation of the relation to the octanol - water partition coefficient.

Department of Chemical and Biochemical Engineering  
Period: 01/01/1998 → 31/12/1998  
Number of participants: 1  
Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

**Prediction of Phase Equilibria and Liquid Phase Nonideality (A.5)**  
To use molecular mechanics methods to estimate parameters in models, which can be used to calculate phase equilibria in nonideal systems.

Department of Chemical and Biochemical Engineering  
Period: 01/01/1998 → 31/12/1998  
Number of participants: 1  
Project Manager, organisational:
Rasmussen, Peter (Intern)

**Recovery processes (C.7)**  
Experimental and theoretical investigations of oil recovery processes with emphasis on low permeable reservoir rocks.

Department of Chemical and Biochemical Engineering  
Period: 01/01/1998 → 31/12/1998  
Number of participants: 8  
Project participant:
Mogensen, Kristian (Intern)  
Poulsen, Søren (Intern)  
Dang, Tran Thuong (Intern)  
Poulsen, Susanne (Intern)  
Shapiro, Alexander (Intern)  
Ivar Andersen, Simon (Intern)  
Dandekar, Abhijit (Intern)  
Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

**Simulation of IOR/EOR with advanced thermodynamic models (C.8)**  

Department of Chemical and Biochemical Engineering  
Period: 01/01/1998 → 31/12/1998  
Number of participants: 3  
Project participant:
Jørgensen, Marianne (Intern)  
Christensen, Jes Reimer ( Intern)  
Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

**Structuring of multiphase polymer systems**  
The project consists of two subprojects: Tayloring of bicontinuous phase structure during flow and structure and properties of materials with microporous microstructure.
Supercritical Fluid Separations (D.2)

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 2
Project participant:
Borch-Jensen, Christina (Intern)
Project Manager, organisational:
Mollerup, Jørgen (Intern)

The Effect of Heat Treatment on Pitch Quality (B.3)

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1
Project participant:
Ivar Andersen, Simon (Intern)
Project Manager, organisational:
Mollerup, Jørgen (Intern)

Thermodynamic Properties of Amino Acids in Solution (D.3)
The objective is to write a computer programme that eventually should be able to estimate the parameters for the extended UNIQUAC model as function of pH and salt concentration.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Mollerup, Jørgen (Intern)

Vapor-Liquid Equilibrium (VLE) Measurements (A.1)
- To make accurate VLE measurements on mixtures containing dichloromethane. - To use a new equipment for VL(L)E measurements at pressures up to 150 bar and temperatures up to 200°C for measurements with systems containing DME.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 3
Project participant:
Wax Formation in Reservoir Fluids (C.6)
To measure high pressure solid phase transitions using real fluids and model systems.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 3
Project participant:
Ivar Andersen, Simon (Intern)
Lindeloff, Niels (Intern)

Control of fouling and concentration polarisation during Microfiltration of skim milk

Department of Chemical and Biochemical Engineering
Period: 01/12/1997 → 07/06/2002
Number of participants: 7
Phd Student:
Guerra, Marie Alexandra (Intern)
Supervisor:
Nielsen, E. Waagner (Ekstern)
Rasmussen, Alan (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Adler-Nissen, Jens (Intern)
Madsen, Rud Frik (Ekstern)
Qvist, Karsten (Intern)

Effekt af varmebehandling på begkvalitet

Department of Chemical and Biochemical Engineering
Period: 01/12/1997 → 14/03/2001
Number of participants: 6
Phd Student:
Ascanius, Birgit Elkjær (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Ivar Andersen, Simon (Intern)
Examiner:
Østergaard, Knud (Intern)
Stokke, Per (Ekstern)
Øye, Harald A. (Ekstern)
Project: PhD

**Fermentering og oprensning af C-5 kulhydrater til mælkesyre**

Department of Chemical and Biochemical Engineering  
Period: 01/12/1997 → 17/02/2003  
Number of participants: 6  
PhD Student:  
Garde, Arvid (Intern)  
Supervisor:  
Ahring, Birgitte Kiær (Intern)  
Main Supervisor:  
Jonsson, Gunnar Eigil (Intern)  
Examiner:  
Villadsen, John (Intern)  
Kristensen, Steen (Ekstern)  
Norddahl, Birgir (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Ansat ekstern  
Project: PhD

**Production of novel plasmid vectors for gene therapy and DNA vaccine applications**

Department of Chemical and Biochemical Engineering  
Period: 01/12/1997 → 05/02/2002  
Number of participants: 6  
PhD Student:  
Theodossiou, Irini (Intern)  
Supervisor:  
Thomas, Owen R. T. (Intern)  
Main Supervisor:  
Villadsen, John (Intern)  
Examiner:  
Jonsson, Gunnar Eigil (Intern)  
Johansen, Jesper Sonne (Ekstern)  
Müller, Markus-Helmut (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Eksternt EU-finansieret  
Project: PhD

**Biologically Based Packaging Materials for Foods**

The objective is to initiate development of a new generation of biologically based packaging materials for selected foods (fruits, vegetables, fresh meats, and dairy products). These materials will be based on starch and microbial polymers. All relevant food quality parameters describing the physical, chemical and microbial quality of package foods will be examined and used to evaluate the packaging materials. Additionally, it will be used for further development of biopolymers. The research activities encompass the whole production chain from selection of raw material, through the processing of the bio-based materials, and finally the investigations of the suitability as food packaging material.

Department of Biotechnology  
Department of Chemical and Biochemical Engineering  
Rise National Laboratory for Sustainable Energy  
Royal Veterinary and Agricultural University  
Danish Technological Institute  
SUC Institute of Biomass Utilization and Biorefinery
Period: 01/10/1997 → 30/06/2001
Number of participants: 2
Project participant:
Bergenholtz, Karina P. (Intern)
Project Manager, organisational:
Nielsen, Per Væggemose (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,991,976.00 Danish Kroner

Fremstilling af nano-partikler og nano-porøse materialer ved aerosolmetoder
Department of Chemical and Biochemical Engineering
Period: 01/10/1997 → 12/07/2001
Number of participants: 6
Phd Student:
Andersen, Henrik (Intern)
Supervisor:
Livbjerg, Hans (Intern)
Main Supervisor:
Wedel, Stig (Ekstern)
Examiner:
Christensen, Kurt Agerbæk (Ekstern)
Høj, Jakob Weiland (Intern)
Jonsson, Gunnar Eigil (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp

Integrated approach to computer aided process synthesis
Department of Chemical and Biochemical Engineering
Period: 01/10/1997 → 20/09/2002
Number of participants: 5
Phd Student:
Hostrup, Martin (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Aasbeg-Petersen, Kim (Ekstern)
Pistikopoulos, Stratos (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU

Integrated system for design and analysis of pharmaceutical, biochemical, and fine-chemical processes with electrolyte systems
Department of Chemical and Biochemical Engineering
Period: 01/09/1997 → 06/04/2001
Number of participants: 4
Phd Student:
Takano, Kiyoteru (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Wiebe, Lars (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden International Finan-SU
Project: PhD

**Kolloide egenskaber af asfaltene i olier**
Department of Chemical and Biochemical Engineering
Period: 01/08/1997 → 09/07/2001
Number of participants: 6
Phd Student:
Pedersen, Carsten (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Ivar Andersen, Simon (Intern)
Examiner:
Thomsen, Kaj (Intern)
Buckley, Jill S. (Ekstern)
Knudsen, Kim (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

**Metabolic engineering of the pyruvate metabolism in Lactococcus lactis**
Department of Chemical and Biochemical Engineering
Period: 01/08/1997 → 09/11/2000
Number of participants: 2
Phd Student:
Melchiorsen, Claus Rix (Intern)
Main Supervisor:
Villadsen, John (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

**Modellering af elektrisk drevne membranprocesser**
Department of Chemical and Biochemical Engineering
Period: 01/08/1997 → 27/05/2003
Number of participants: 4
Phd Student:
Rype, Jens-Ulrik (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Jacobsen, Torben (Ekstern)
Kristensen, Steen (Ekstern)

**Financing sources**
Oil recovery processes
Department of Chemical and Biochemical Engineering
Period: 01/08/1997 → 14/09/2001
Number of participants: 5
Phd Student:
Poulsen, Susanne (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Foged, Niels Tækker (Intern)
Patzek, Tadeusz W. (Ekstern)
Reffstrup, Jan Otto (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Optimizing control of integrated processes
Department of Chemical and Biochemical Engineering
Period: 01/08/1997 → 03/06/2005
Number of participants: 5
Phd Student:
Jørgensen, John Bagterp (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Poulsen, Niels Kjølstad (Intern)
Marquardt, Wolfgang (Ekstern)
Strand, Stig (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Center-Finansieret-SU
Project: PhD

Raman Spectroscopy Analysis of Phase Equilibria
Phase Equilibria in multicomponent systems, e.g. in fuels, oil and gasses, are studied by Raman and IR spectroscopy. The project is a ph.d. project for Susanne Brunsgaard Hansen, supported by The National Oil and Gas Company of Denmark, The Nordic Energy Research Program and The Danish Technical Research Council.

Department of Chemistry
Department of Chemical and Biochemical Engineering
Center for Energy Resources Engineering
DONG Energy A/S

Nordiske Energiforskningsprogram
Period: 01/07/1997 → 30/01/2001
Number of participants: 3
Project participant:
Hansen, Susanne Brunsgaard (Intern)
Stenby, Erling Halfdan (Intern)
Berg, Rolf W. (Intern)
**Financing sources**
Source: Unknown
Name of research programme: Ukendt
Amount: 648,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 274,485.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 100,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 150,000.00 Danish Kroner

**Pyrolyse og forbrænding af biomasse**
Department of Chemical and Biochemical Engineering
Period: 01/06/1997 → 19/09/2001
Number of participants: 5
Phd Student:
Stenseng, Mette (Intern)
Supervisor:
Jensen, Anker Degn (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Hansen, Peter F. Binderup (Ekstern)
Mogensen, Gurli (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

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**A.1 Activity coefficient models**
The objective of this project is to develop new models that will enhance the application range of group contribution approaches. Currently, we have two active projects in this area. The first is a PhD-level project whose objective is to develop a second-order model for estimation of liquid phase activity coefficients considering UNIFAC as the basic (first-order) model. The principal idea is that through the addition of a second-order term, some of the well-known limitations of the UNIFAC model can be overcome. Since the UNIFAC (first-order) groups are limited in terms of the molecular structural information they can provide, they are also limited to the contributions they can provide to the corresponding activity coefficient value of the molecule in a liquid mixture with other molecules. The second-order term, which is added to the original first order expression, has been derived through Taylor series expansion of the first-order model with respect to the group interaction parameters (second-order). The second project in this section deals with the development of a software library containing a large collection of activity coefficient models that can be used for various applications (in-house or external). Activity coefficient models suitable for mixtures with electrolyte systems are also being studied.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 4
Project participant:
Abildskov, Jens (Ekstern)
Takano, Kiyotetu (Intern)
Jensen, Anne Krogh (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

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**A.2 Pure component property estimation methods and software**
In the area of pure component property estimation methods, we have concentrated our efforts on the development of new methods for properties not covered by us before, and, in the extension of existing methods to also cover compounds with complex molecular structures (heterocyclic-ring, multi-ring, and large molecules). The properties have been classified as
primary (can be estimated only from molecular structural information), secondary (can be estimated from other known properties) and functional (depends on temperature, pressure and/or composition). New methods have been developed mainly for primary properties. For secondary properties, well known and well tested correlations have been programmed and included in the property prediction software (ProPred). For functional properties, two options have been developed. In the first option, given the data and a function, the function parameters are determined through regression. In the second option, data are generated through an equation of state or corresponding states model and then fitted to a specified function. In the primary property estimation area, the melting point method of Constantinou and Gani is being revised and a new model for estimation of the standard heats of fusion is being developed. For primary properties, the Constantinou & Gani method as well as the Joback method has been added in ProPred. The primary property estimation methods are also being extended to polymers. In the secondary property area, a large collection of methods has been tested and added to ProPred (properties such as solubility parameter, refractive index, and many more have been added). A new atom contribution method (proposed by Wilson) is being currently added to ProPred. In the functional property area, generation and regression of temperature dependent data for vapour pressures is now possible. Other properties to be included soon are surface tension, viscosity, density, thermal conductivity and heat capacity.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Harper, Peter Mathias (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

A.3 Computation of chemical and/or physical equilibrium

Computation of phase equilibrium (with or without chemical reaction) continues to be an important part of our research effort. This is because in our opinion, phase diagram based design/analysis provide a simple yet accurate way of visualising the operation of processes where phase equilibrium has a significant role. A major effort has been devoted to the computation of simultaneous chemical and physical equilibrium based on a new algorithm (PhD-thesis of Eduardo Perez-Cisneros, 1997). Employing an element-approach, the new algorithm reduces the dimension of the problem, thereby, providing the visualisation of the phase behaviour for multi-component systems in two- or three-dimensional phase diagrams. The new algorithm is also able to compute the presence of "element" reactive azeotropes. A unique feature of the new algorithm is that, the computation of the element-based chemical and physical equilibrium problem is identical to that of computation of component based physical equilibrium problem. CAPEC has earlier developed a collection of robust and efficient physical equilibrium computational modules (such as location of binary azeotropes, SLE and high pressure VLE). In the area of electrolytes, CAPEC has started a new PhD-level project where issues related to prediction of activity coefficients for calculation of PH and solubility diagrams for mixtures with electrolyte systems are being addressed. Known activity coefficients are being examined for their applicability and the unavailable model parameters are being estimated through a developed parameter estimation program. Since data for many electrolyte systems are limited to a few measured points, a thorough analysis of the sensitivity of the activity coefficient model parameters is being made. Preliminary results from the sensitivity analysis show that not all the model parameters need to be estimated as only a few affects the activity coefficient value.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 4
Project participant:
Jensen, Anne Krogh (Intern)
Takano, Kiyoteru (Intern)
Hostrup, Martin (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

A.4 Data visualisation and parameter estimation

A computer aided system targeted on the identification of relationships between compound structure/class and properties, maintenance of a validated sets of experimental data and assisting in the development of new group contribution methods is under development. The software, called DATA, is currently able to: Show single component properties, and allow the user to add data to an existing database or to create a new database. Show properties for a subset of compounds (chosen by the user), with tabular presentation and with graphical presentation. Show mixture properties (tabular presentation and graphical presentation). Currently, the available mixture properties are infinite dilution activity coefficients and VLE-data. A small database, containing carefully screened and selected experimental data, is part of the DATA software. Since all model development activities require parameter estimation, another project in this section deals with the development of general parameter estimation software that will be used in all model development work. The future plans in this area is to add more properties (pure component and mixture) and integrate DATA to a parameter estimation program so that new
property estimation method can be developed as well as existing model parameters can be re-estimated with new data or with selected sub-sets of data.

A.5 Databank management and access tools
Access to data and parameters of various kinds, is of key importance in order to perform almost any task in CAPE. In order to ease the task of database maintenance and improve access times, storage and retrieval of data, it is desirable to use advanced database features and formats. The goal is to develop one single structure capable of fulfilling the data needs of all programs developed within CAPEC and for use within ICAS (see program research E and CAPEC software). A study of the needs and demands of the various programs within CAPEC has been started and minor tests of database engines and access tool have been performed. Current and future plans include the formalisation of the database/databank structure and the development of the needed routine library for data access and maintenance.

A. Correlation/prediction of thermo-physical and phase equilibrium properties

B.1 Integrated process simulation
The objective of this project is to develop an integrated approach to process simulation. Process simulation needs differ significantly with respect to problem type, for example, simulation for design or simulation for control require different tools. Also, the modelling and simulation problem can be quite different with respect to the type of mixture present in the system. For example, models for mixtures with electrolytes are quite different than models for mixtures with normal fluids. In order to achieve a large application range in terms of process as well as in terms of mixtures, it is necessary for the simulation system to be versatile and flexible without sacrificing computational efficiency and accuracy. Simulation strategy defines the appropriate method of solution for a specified simulation problem (steady state simulation, dynamic simulation, simulation for design, etc.). A simulation system capable of steady state and dynamic modes of simulation with equation oriented as well as modular approaches has been developed and incorporated into ICAS (see research program E). A biochemical process simulation feature has also been added. It is possible to simulate the behaviour of the biochemical process in various modes of operation (batch, fed-batch and continuous). Current and future work plan include the development of a number of features to our simulation approach in order to be able to solve a wide range of problems with the same set of tools. Work on the following projects has been started: Development of a switching policy between the equation oriented approach and the modular approach for any simulation problem; Mixed mode simulation; Generation of steady state and/or dynamic simulation features from the same model library; Inclusion of new unit operation modules; Development of CAPE-OPEN standards for connection with external modules.
B.2 Modelling and simulation of membrane-based separation processes

In recent years membrane-based separation systems have been employed successfully for a number of gas and liquid separation tasks. Besides end-of-pipe installations, membrane systems are more and more used as part of a complex flowsheet in combination with other unit operations. If the boundary conditions are in favour of a membrane system, a membrane plant offers several advantages because of its modular structure, low energy consumption and ease of operation. Membrane modules are generally not included in commercial process simulators as standard unit operations. The objective of this project is to develop mathematical models for membrane-based separation processes. Two separation processes have been considered: gas separation and liquid separation by membrane distillation. A mathematical model for membrane gas separators operated in co-, counter- or crosscurrent flow mode has been developed. The model consists of differential material balance equations and optionally differential pressure drop equations on both sides of the membrane. Furthermore, the non-ideality of the gas phases can be taken into account via an equation of state. For membrane distillation, a rate-based model has been developed for the co-current flow mode. Current and future work includes testing of the developed algorithm against industrial problems (gas separation) and against known case studies (liquid separation by membrane distillation). Professor Michael L. Michelsen, KT-DTU and Professor Gunnar Johnson, KT-DTU are collaborating partners in this project.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 4
Project participant:
Tessendorf, Stefan (Intern)
Michelsen, Michael L. (Ekstern)
Jonsson, Gunnar (Ekstern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

B.3 Modelling and simulation of fixed-bed reactors

Gas phase fixed bed reactors constitute one of the most common reactor classes in industry. However fixed bed reactors are generally not included as standard modules in commercial simulation packages. The goal of this project is to develop models for fixed bed reactors with the purpose of understanding non-linear dynamic behaviour. Three reactor types are considered. Hereof two types are continuously operated fixed bed reactors which in one case is indirectly cooled and contain two or more catalyst beds with one or more inter-bed heat exchangers and in the other case is directly cooled by heat exchange through the catalyst tube wall. The third type is a periodically operated fixed bed reactor containing multiple beds. This reactor type is used for heat regenerative oxidation of a dilute mixture of combustible gases. With the given purpose simple models should be developed. For an indirectly cooled ammonia reactor a dynamic pseudo-homogeneous model of the catalyst bed with only 3 partial differential equations has been developed. Simulations with the model show very good agreement with a heterogeneous model with 6 PDEs. One inter-bed heat exchanger is modelled with 4 ordinary differential equations and good agreement has been achieved when compared with more complex models also for varying flow rates. Models have also been derived on a similar basis for a directly cooled methanol reactor and for a periodically operated multi-bed regenerative reactor with a single oxidation reaction. Future work include performing bifurcation analysis for a part of an ammonia reactor where the first bed is coupled to an inter-bed heat exchanger which effectively acts as a feed-effluent heat exchanger. This system thus includes energy recycle.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 3
Project participant:
Recke, Bodil (Intern)
Keldebaek, Morten (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

B.4 Modelling and simulation of particulate transport in rotary kiln

Particulate transport in continuous rotary drums is widely used in the chemical and metallurgical industries. The applications include as diverse areas as mixing, drying and reaction. However no satisfactory model has been proposed for this type of operation and is thus not generally available in standard simulators. The model development is based upon a detailed experimental study of particle movement in a two-dimensional disk and in rotary cylinders. Upon this basis a
nonlinear partial differential equation model is developed for the normal rolling transport of particles. The basic idea is that particles roll on the bed surface, but spend most of the time being transported by rotation inside the particle bed. This model demonstrates very good agreement with experimental measurements.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 1
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

B.5 Modelling and simulation reactive separation processes
The work in this research project is currently focused on cultivations of filamentous fungi and of Saccharomyces cerevisiae. In the first project, structured process models are being developed to study key factors in the submerged cultures of filamentous fungi, i.e. Aspergillus oryzae for production of -amylase in high performance bioreactors. The simulation results with the developed models have been compared with experimental data. The results indicate that the influence of oxygen limitation on the process depends on the specific growth rate. The maximum specific productivity for -amylase is reached when the specific growth rate is about 0.15 h⁻¹ (Dp). For specific growth rates below Dp, oxygen limitation takes place simultaneously on both biomass formation and enzyme production. For growth rates above Dp, a decoupling between the limitation on biomass formation and enzyme production is observed. Amylase production becomes more sensitive to the low levels of oxygen and decreases even though the biomass concentration remains constant. Present and future work in this project is to improve the feature for estimation of model parameters, validation of the model by obtaining more experimental fermentation data.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 3
Project participant:
Lei, Frede (Intern)
Pedersen, Kurt (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

B.6 Modelling and simulation reactive separation processes
Equilibrium based models Rate based models

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Hostrup, Martin (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

B.7 Modelling and simulation of biological waste water treatment processes
Biological phosphorous removal

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 3
Project participant:
Meinhold, Jens (Intern)
Krühne, Ulrich (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

B.8 Modelling and simulation of electrolyte processes
Crystallisation (mixed solvents)
B.9 Real-time refinery predictive models

The high quality, and environmental friendly demands for gasoline products, combined with strong market competition and downward tendency of gasoline consumption, encourages the refiners to effectively reduce the amount of "give-away" for their gasoline products. On that account, minimisation of productivity cost function subject to optimum qualities of naphtha products from reforming and isomerization processes, together with gasoline blending, is of significant economical benefit. The main objective of the Real-time Refinery Optimisation System (ROS) is to determine the targets for the process control system in such a way that the needed quantities of the different gasoline types can be produced on-time with the desired specifications in an economically optimal manner. An important basis for ROS is development of accurate predictive models for qualities of naphtha products, especially from reforming and isomerization processes. These models are mainly for prediction of Research Octane Number (RON), Reid Vapour Pressure (RVP), concentration of aromatic compounds, e.g. benzene, in the products, and ASTM distillation curve. The types of predictive models in this work are ARX and ARMAX (Auto Regressive Moving Average with external input), i.e., parametric input-output representations. Since quality measurements are either expensive or delayed, only a limited number is available. Hence the need for predictive models is eminent.

B. Process modelling, simulation and identification

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 1
Project Manager, organisational: Jørgensen, Sten Bay (Intern)
Project

C.1 Process synthesis with thermodynamic and physical insights

Similar synthesis (flowsheet generation) algorithms are also being developed for pharmaceutical and biochemical processes. Since, compared to the chemical processes, these processes are considerably different, the synthesis algorithm needs modifications. This is primarily because many of the needed properties may not be available. Therefore, new definitions of relationships between separation techniques and process design independent of the properties need to be developed. It has been possible to graphically generate feasible process flowsheets together with the corresponding conditions of operation through the use of solubility diagrams of mixtures with electrolyte systems. These methods are now being converted into computer aided synthesis and design techniques. Research on hybrid separation processes has been started. The principle of hybridisation has been defined as the use of two or more separation techniques at their highest separation efficiencies in order to perform a desirable separation. As an example, consider the separation of aqueous azeotropic mixtures. By conventional distillation alone it is not possible to obtain pure products because of the azeotrope. However, for those azeotropes that are at the low concentration range of water, pervaporation is highly efficient to remove the last amounts of water (starting at the azeotropic point and ending at the pure product). The objective of the project is to develop computer aided synthesis and design techniques for generation of hybrid separation schemes that are energy efficient and environmentally benign. This project is funded by the European Union and has partners from UK, Belgium and Greece.
C.2 Computer Aided Molecular Design (CAMD)

Computer aided molecular design (CAMD) provides a means for determining molecules having a desirable set of physico-chemical properties. As the physico-chemical properties are directly or indirectly related to the structure of the molecule(s), methodologies for CAMD are typically based on "exploiting" these relationships. A multi-level approach is currently under development. In this approach each level has its own generation and testing steps. The results from each level "trickle down" to the next level. This ensures that the size of the combinatorial problem is continuously held at a level where it can be handled effectively without any so-called "combinatorial explosion". Furthermore, by having the most time consuming operations at the higher levels where the remaining candidates are the most promising, efficiency with respect to execution time is naturally obtained. Since the actual calculation/estimation of the properties is done using purely predictive methods, the accuracy, speed and applicability (with respect to level of detail needed in the molecule description) are aspects which have to be taken into considerations when selecting how and where to apply the various methods. Note that there may be several different available methods. It is possible to design molecules with a significant level of detail (down to a 3-dimensional model on atomic level) without suffering from combinatorial explosion and without sacrifice of computational accuracy. Once a 3-dimensional model is obtained results can be exported directly into molecular modelling programs for further analysis. Current work is also investigating the developing of an interactive CAMD feature. The objective here is to design the molecule with desirable properties through interaction with the user.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Harper, Peter Mathias (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

C.3 Design and analysis

Aspects of design and analysis of separation processes such as azeotropic distillation, reactive distillation, membrane-based gas separation, crystallisation have been investigated. Also, the design and analysis of various types of reactor operations have been investigated. Operation of azeotropic distillation and fixed bed reactors were studied in detail. In the case of reactive distillation, the element-based approach used for modelling these processes permitted the development of a suite of simple graphical design/analysis techniques. A unique feature of these techniques is that an element-based reactive distillation is identical to component-based non-reactive distillation. Therefore, by incorporating the element transformations on the well known component-based non-reactive distillation design techniques (such as the McCabe-Thiele method, the residue curves, distillation boundaries, the Lewis-Matheson method, etc.), it has been possible to employ these techniques also for design of reactive distillation. In the membrane-based separation processes, use of orthogonal collocation method permitted the simultaneous computation of analytical sensitivities, that is, derivatives of the model output variables with respect to any parameter in the equation system. This resulted in an efficient and versatile module that can be used for simulation and design as well as for optimisation and parameter estimation calculations.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 8
Project participant:
Recke, Bodil (Intern)
Andersen, Torben Ravn (Intern)
Hostrup, Martin (Intern)
Takano, Kiyoteru (Intern)
Tessendorf, Stefan (Intern)
Lei, Frede (Intern)
Pedersen, Kurt (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)
C. Process synthesis, process/product design and analysis

Three areas of research have received attention during the last twelve months. The objective of the first project is the development of a generalised methodology for generation of physically feasible process flowsheets. The thermodynamic insights based synthesis method developed earlier by Jaksland (PhD thesis Cecilia Jaksland, 1996) is further developed to include new definitions of properties-separation process relationships, to include new properties and separation processes and to include rules which enable the application of the synthesis algorithm when properties are not available. Also, the new algorithm can include the reactor in the flowsheet. The methodology employs a four-step procedure: a) mixture analysis, b) calculation of component property ratios, c) using the results of the previous steps to find the feasible separation techniques and d) listing the possible alternatives of the feasible separation techniques.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

D.1 Statistical process monitoring and optimisation

Readily available online measurement data can be effectively used in industrial practice for monitoring process performance. The statistical tools enables unveiling multivariate behaviours and thus to map the performance down into a space of comparatively low dimensionality where supervision is greatly facilitated. In this project research aspects of monitoring continuous and semi-continuous processes are considered. On continuous processes the project deals with multivariate monitoring of multi-modal processes based on principal component analysis (PCA). For continuous chemical process plants operating at one operation mode this technique has been proven to work well. The sound statistical basis of the technique is however lost when the monitored process has more than one operation mode. The result is a reduction is the fault detection sensitivity. The purpose of the project is to develop approaches to enhance the monitoring capability of the technique when monitoring processes with more than one operation mode. It is intended to do this by using localised PCA representations, either based on a number of pre-determined representations or by constant updates of the representation using exponential weighted moving average. The analysis will be performed on data from the energy-integrated distillation column located at CAPEC, DTU. Fed-batch fermentation processes are time consuming and difficult to model using first principle models and these models are difficult to apply in production. Instead the process can be modelled by using data based modelling. The fault diagnosis utilises a statistical model based on either PCA (principal components analysis) or PLS (projection to latent structures) to describe normal behaviour. Deviations from normal conditions can easily be detected and displayed to the process operators, which leaves them time to take action to eliminate the fault. The methodology has been demonstrated on a fermentation process.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Gregersen, Lars (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

D.2 Real-time optimising control

Issues in real time optimisation are relevant in many instances of process operation. In this project two instances are investigated. One is in scheduling plant operations in accord with market demands and raw material availability thus providing set points for the control loops. The other deals with operating semi-continuous or fed-batch processes where the feeding profiles are determined to optimise the process productivity under the loads of changing raw material and catalyst properties. A methodology for simultaneous dynamic optimisation of gasoline production and blending in response to market demands of a refinery is being developed. The optimisation decides the set points for the refinery operations as well as the blending recipe such that profit is maximised several time periods into the future. As such the optimisation program has strong similarities to the receding horizon controller employed in model predictive control. The main model requirements are that the gasoline blending model is piecewise linear and that reactors and fractionators in the gasoline production plant are restricted to a finite set of possible operation points. Using these simplifying but realistic assumptions the model can be formulated as a large-scale MILP model. This model is solved using CPLEX. The actual refinery operation profitability of this approach remains to be explored. In control of semi-continuous or fed-batch processes the first engineering principle models are time varying and non-linear thus the resulting control problem becomes a rather complicated non-linear optimisation which however often can be solved within reasonable computational time. In this project optimising control of filamentous fungi cultivations and of Saccharomyces cerevisiae cultivations will be investigated. The applied cultivation models will be structured models for the organisms.
D.3 Operational implications of optimality
The purpose of this research project is to explore the operational and controllability properties of integrated processes and processes designed to operate at optimal profit. The focus is to develop operating strategies for highly integrated processes. It is well known for simple processes in which the optimum is unconstrained, that mathematically the profit is uncontrollable near the optimal profit if only the product quality itself or some related variable is measured. On the other hand if all states are always measured or available, the maximum profit can be controlled. For integrated process the process non-linearities imply that these processes are often uncontrollable by simple output feedback.

D.4 Non-linear dynamics and control
Near optimal productivity many plants exhibit complex non-linear behaviours which often give rise to complex control problems. The objectives of this project are to elucidate some typical complex behaviours encountered in chemical processes and to investigate measures for preventing undesirable behaviour through modified process or control design. Several cases have been preliminarily investigated as far as the first purpose is concerned and complex behaviours have been encountered in, e.g. recycle fixed bed reactors, continuous cultivation reactors and in azeotropic distillation sequences. The future research will also include investigation of how to deal with the encountered types of non-linear behaviours including non-linear control designs.

D.5 Control of biological waste water treatment process
Biological wastewater treatment processes using activated sludge may be operated as a periodic cycled plant to enable better possibilities for manipulating the process. The operational task is complicated by the desire to remove Carbon, Nitrogen and Phosphorous to fulfill requirements upon effluent quality. These requirements render this task a typical multivariable control problem. The number of handles in conventional waste water plants is rather limited, therefore there is considerable interest in exploiting the additional degrees of freedom available in periodically operated plants. The activated sludge process consists of two reactors alternating between aerobic and anoxic conditions. As this process is operated periodically it is highly non-linear. In a first phase of this project a period-to-period linearized model of the plant will be investigated concerning its ability to predict the inter-periodic plant performance. Subsequently, both model verification and state estimation will be investigated. One key aspect is the model detail that is required to obtain reliable predictions several periods ahead. Subsequently it is intended to investigate the achievable inter-periodic control performance of the plant using a linear state space MPC controller.
D.6 Implementation of control into ICAS
The goal of the project is to introduce control aspects into the dynamic simulator included in ICAS. The project includes two parts: 1. Dynamic control: To provide the facilities for specification of simple control loops in dynamic simulation within ICAS. 2. Process analysis: Tools for linearization will be developed for the purpose of implementing tools for process analysis, such as SVD, RGA, DC-maps etc. The latter aspect will be used in connection with control structuring which is one active research area within process control. Selection of a control structure concerns deciding which variables to manipulate and which variables to control in a multi-loop control structure. Frequency dependent RGA and SVD analysis has been applied. Also a novel method formulating the control structure selection as an assignment problem or MILP problem using a modified steady-state RGA in the objective function has been developed. This research project aims at synthesising a control structure given the design of a plant.

D.7 Development of toolbox for linear and non-linear MPC
The research concerning model predictive control focuses on development of toolboxes for both ICAS and Matlab. The model predictive controllers are based on a receding horizon principle in which the variables that can be manipulated are controlled at each sampling time by solving a quadratic or linear optimisation problem. The linear model predictive controller is in state space form and provides guaranteed nominal stability. A Kalman-filter is used for state estimation from the measurements. The linear models are identified by subspace identification. Stability properties are also investigated. The model predictive control methodologies developed has been applied to a number of periodic operating processes, i.e. to control a simulated industrial flow swing reactor, and is being investigated for control of an activated sludge process. Future work focuses around the non-linear model state estimation and predictive controller. Currently the methodology is based upon a first-principles model and either an extended Kalman-filter or a receding horizon estimator for estimation of the states given the outputs. Approaches for utilising the special structure of the optimisation problem are being investigated.
E.1 Process Integration
A project concerning development of a simulation tool (steady state as well as dynamic) for Petlyuk distillation columns has been initiated. The objective for development of this tool is to study the operation of integrated distillation trains. Distillation column configuration for the separation of azeotropic mixtures continues to attract industrial and academic researchers. For heterogeneous azeotropic mixture separation, the advantages and disadvantages of the "direct-sequence" and the "indirect-sequence" have been studied at CAPEC. The conditions, under which the undesirable effects of multiple solutions can be avoided, have been identified for various design/operational alternatives.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 3
Project participant:
Andersen, Torben Ravn (Intern)
Jørgensen, Sten Bay (Intern)

Project Manager, organisational:
Gani, Rafiqul (Intern)

E.2 System (Tools) Integration
ICAS: Integrated Computer Aided System Solutions of process integration problems require an integrated set of tools. There is a demand for tools that will enable the engineer to directly transfer information between various phases of process design, process analysis, and process optimisation. Therefore, an integrated computer aided system for process modelling, simulation, design, synthesis and analysis has been developed. This system includes a simulation (steady state and dynamic) engine and tools for physical properties estimation, process/product synthesis and process/product design. The total system, called ICAS, has been evaluated against various test problems. A major part of the tools integration within ICAS has been developed through a PhD-project (PhD thesis of Anne K. Jensen, May 1998), where, emphasis has also been given to the development of a computer aided modelling system. The model generation feature in ICAS consists of a generic modelling language for interactive definition of new building objects and a knowledge-based modelling language that apply rules in order to create new building objects. The methodology for creation of building objects is essentially based on information related to definition of control shells (boundary, physical description of the interior, and interactions between the shell and the surrounding). From the definition of the control shell, the computer aided modelling system generates the model equations describing the control shell. In addition to the creation of new objects, a system for graphical aggregation of the building object into a composite model has also been developed. Finally, integration of the model generator to a process simulator allows direct simulation with the generated model (the appropriate code for the simulator is generated by the model generation feature).

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 7
Project participant:
Jensen, Anne Krogh (Intern)
Russel, Boris Mariboe (Intern)
Harper, Peter Mathias (Intern)
Hostrup, Martin (Intern)
Jørgensen, John Bagterp (Intern)
Andersen, Torben Ravn (Intern)

Project Manager, organisational:
Gani, Rafiqul (Intern)

E.3 Integrated Algorithms
Integration of process synthesis, design and control In design of continuous process flowsheets, it is desirable to limit the variety of possible flowsheets as early as possible. If screening of flowsheets is done entirely on the basis of steady state economics, it will often lead to solutions where dynamic behaviour causes the final plant to be difficult to control (or even impossible to control). It is therefore desirable to have an integrated set of tools through which design and control engineers can find feasible flowsheets from steady state information alone, at an early stage of the project. The plan for this project is to develop an integrated approach to design, synthesis and control of chemical processes on the basis of thermodynamic insights. The goal is to present a methodology which leads to a flowsheet of a process where aspects of design (condition of operation), synthesis (choice of unit operations) and operability (energy requirements, controllability, environmental impact, etc.) are addressed in an integrated manner. This methodology will be applicable to design of new processes or for determining appropriate alternatives for existing processes (retrofit problems). Inclusion of all sub problems into the objective of the design (for the optimal solution) will provide a multi parametric function. The trade off
between the various terms will be analyzed through "trade off curves". Thermodynamic insights will help to understand these curves and to apply them in the integrated approach.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 3
Project participant:
Lewin, D.R. (Ekstern)
O'Connell, J.P. (Ekstern)
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

E. Process and Tools Integration

F.1 Numerical Methods Collection
Optimisation techniques DAE-solvers. The objective of this project is collect and implement numerical methods suitable for inclusion into the solver toolbox of ICAS. ICAS requires numerical routines for algebraic equations solving, differential and algebraic equation solving, partial differential equation (plus algebraic equations) solving, optimisation methods and many more. A project to implement, update and validate optimisation methods and DAE-solvers has been started. NLP as well as MINLP methods are being implemented under optimisation techniques. Index-one DAE-solvers (with initialisation feature) with options for switching between stiff/non-stiff methods, dense/sparse methods and DAE/ODE modes of simulation are being investigated.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Jensen, Anne Krogh (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

F.2 Initialisation for large problems
Distillation simulation Solution of very large steady state simulation problems (more than 10000 equations and variables) may require very long computing times, even with the fastest computers. If steady state simulation is performed for process optimisation, even longer computing times may be necessary. One way of reducing the computing times is to provide better initial estimates so that a faster convergence to the solution can be obtained for the simulation/optimisation problem. For single and multiple column distillation problems, an efficient initialisation procedure has been developed and validated with several test examples. Large reduction of computational times have been achieved by first solving a reduced problem. A unique feature of the reduced problem is that it represents a linear set of algebraic equations and the key distillation model variables (for the large problem) is predicted with reasonable accuracy, thereby, providing very good initial estimates. The applicability of this approach for other problems will be investigated in future.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

F.3 Simulation strategy
Flowsheet decomposition and equation ordering Solution of flowsheet simulation problems with the modular approach requires flowsheet decomposition techniques so that the appropriate calculation order can be specified to the solver. The same problem when solved with the equation oriented approach, needs the equations to be ordered (if possible) in a particular manner so that the solution efficiency can be improved. In an integrated approach to process simulation, design
and control, the simulation engine needs to be flexible so that it is possible to move from one mode of simulation to another without much extra work. Also, if simulation engine is provided from two different sources employing two different solution approaches, they may need to interact through a common set of variables. It may also be that in the same process flowsheet, one part is suitable for solution with the modular approach while another part may be suitable for the equation oriented approach. The same may be true for dynamic simulation of a process flowsheet containing dynamic and non-dynamic units. The objective of this project is to determine appropriate simulation strategies for the simulation engine so that mixed mode (steady state/dynamic, equation oriented/modular, ODE/DAE) simulation is possible with increased solution efficiency and robustness. Since all simulation problems need the same flowsheet topology information, this information may also be used to link flowsheet decomposition and equation ordering. ICAS (see program E) has a built-in feature for defining any problem specific simulation strategy. Current and future work will take these ideas further with a view to the development of generalized strategies of wide application range.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 3
Project participant:
Jensen, Anne Krogh (Intern)
Russel, Boris Mariboe (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

F. Numerical and Computational Aspects

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

G. Process Hazards and Safety

Design and Control of Safety Critical Processes This program is new and under development. The purpose of this project is to establish methods for evaluation of process safety, which are based upon known non-linear process behaviour near safety critical operating conditions. One methodology has been developed and evaluated on batch, semibatch or continuous homogeneous reactors with potential for thermal runaway. The initial aim is to clarify the safety margin imbedded in conventional safety related design rules for safety critical reactors. A further aim is to investigate possible benefits from control.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Recke, Bodil (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

A Multi-phase, Multi-level Framework for Computer aided Molecular Design

Department of Chemical and Biochemical Engineering
Period: 01/02/1997 → 25/07/2000
Number of participants: 4
Phd Student:
Harper, Peter Mathias (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Control of Biological Waste Water Treatment Plants

Department of Chemical and Biochemical Engineering

Department of Biotechnology
Period: 01/02/1997 → …
Number of participants: 6
Project participant:
Krühne, Ulrich (Intern)
Løfvall, Jan Michael (Intern)
Søeberg, Henrik (Intern)
Meinhold, Jens (Intern)
Isaacs, Steven Howard (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

Financing sources
Source: Unknown
Name of research programme: Uændt
Amount: 1,091,000.00 Danish Kroner
Project

Gasinjektion i

Department of Chemical and Biochemical Engineering
Period: 01/02/1997 → 31/07/2000
Number of participants: 4
Phd Student:
Jessen, Kristian (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Optimal design og operation af procesintegreret destillation

Department of Chemical and Biochemical Engineering
Period: 01/02/1997 → 24/01/2003
Number of participants: 5
Phd Student:
Andersen, Torben Ravn (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Gani, Rafiquel (Intern)
Andersen, Henrik Weisberg (Ekstern)
Skogestad, Sigurd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD
EFP-97: Fuel Flexibility and Emission Control - By Production of Electricity and Heat and in Energy Intensive Industrial Processes

The Danish energy policy gives a high priority to a good economy, safe supply and environmentally friendly production. Furthermore, the competitive power of Danish industry must be secured. In many years ahead different types of fossil and biofuels will be used in Denmark and abroad. An important condition for fast and effectively switching to new fuels is a good knowledge to these fuels and their characteristic. The goal of the present project is, across technologies, to build up systematic knowledge of the combustion of different fuels and their emission characteristic, so that industry and public authorities may safely use new fuels in an economic and environmentally safe way.

Department of Chemical and Biochemical Engineering
Period: 01/01/1997 → 31/12/1999
Number of participants: 4
Project participant:
Stenseng, Mette (Intern)
Zolin, Alfredo (Intern)
Røjel, Hanne (Intern)
Project Manager, organisational:
Jensen, Anker Degn (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 7,800,000.00 Danish Kroner

Reaktivitet af faste brændsler

Department of Chemical and Biochemical Engineering
Period: 01/01/1997 → 16/10/2001
Number of participants: 6
Phd Student:
Zolin, Alfredo (Intern)
Supervisor:
Jensen, Anker Degn (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Hurt, Robert (Ekstern)
Pedersen, Lars Storm (Intern)
Rosenberg, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

Transition Metal Complex Catalyzed Hydroformylation in Biphasic Reaction Media.

The heterogenization in a mobile phase of a homogeneous hydroformylation catalyst based on rhodium complexes has been established in two ways: 1) A catalytically active complex based on Rh and 3,4-dimethyl-2,4,5-triphenyl -1-phosphanorborna-2,5-dien(DMTPPNOR) was dissolved in an organic liquid phase, which was distributed in the pore system of a solid support (SLP catalyst). 2) The same Rh-complex was made water soluble by sulfonation of the ligand (DMTPPNOR) and the complex was dissolved in water, which was distributed in the pore system of a solid support (SAP-catalyst). The activity of both of these catalysts was monitored by kinetic examination of the gas phase hydroformylation of propene in a plug flow reactor containing a fixed bed of the catalyst. Preliminary tests indicate that the SAP-catalyst is more than twice as active as the SLP-catalyst, and that the activity may be further increased by careful hamonization of the P/Rh-ratio in the SAP-catalyst. Another perspective is that the SAP-catalyst - contrary to the SLP-catalyst - should be usable in a liquid-flow system (for hydroformylation og higher alkenes), because the catalytic complex is not soluble in the organic reactant stream, i.e. the catalyzed reaction is running at the interphase between the organic reactant/product stream and the aqueous phase containing the catalyst.

Department of Chemical and Biochemical Engineering
Period: 01/01/1997 → 31/12/1997
Number of participants: 1
Project Manager, organisational: Hjortkær, Jes (Intern)

**Project**

**Identifikation af kontrolpunkter i mikrobiel metabolisme**

Department of Chemical and Biochemical Engineering
Period: 01/09/1996 → 28/02/2000
Number of participants: 3
Phd Student:
Jensen, Niels B.S. (Intern)
Main Supervisor:
Villadsen, John (Intern)
Examiner:
Adler-Nissen, Jens (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

**Aske. og Belefningsdannelse i Fyringssystemer**

Department of Chemical and Biochemical Engineering
Period: 01/08/1996 → 28/09/2001
Number of participants: 6
Phd Student:
Becerra, Signe V.r.v. (Intern)
Supervisor:
Jappe Frandsen, Flemming (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Dockter, Bruce A. (Ekstern)
Hansen, Peter F. Binderup (Ekstern)
Skrifvars, Bengt-Johan (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

**Emission af kulbrinter fra lean.brun gasmotorer**

Department of Chemical and Biochemical Engineering
Period: 01/08/1996 → 06/09/1999
Number of participants: 4
Phd Student:
Bendtsen, Anders Broe (Intern)
Supervisor:
Glarborg, Peter (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Martens, Harald (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Kandidatstipendium ansat på DT
Modelling of the Ultra- and Microfiltration Process

Membrane processes have been a promising alternative to other separation processes for some time. For instance one separation task within the biotechnological industry is the separation of products (enzymes) from the fermentation broth which furthermore contain cells and cell debris. The separation is carried out using centrifugation which is a batch process and therefore an inherently expensive separation process. This process could be replaced with a continuous membrane process that is microfiltration. The major problem with the replacement is the severe fouling of the membrane one is faced with. This will cause a large decrease in the flux (a 90% decrease compared to the pure water flux has been observed). Due to the fouling an in situ cleaning of the membrane would be very promising technique to prevent the fouling. Such a cleaning method has been developed in the membrane group in collaboration with the membrane group at the Department of Biotechnology. The cleaning method has been named the backshock technique. The microfiltration process in combination with the backshock technique has been successfully applied to industrial liquids like beer and milk. The optimisation of the process has until now been carried out in a more or less empirical way. It would be of great interest to perform the optimisation in a more general way for example with the aid of models for the process.

Department of Chemical and Biochemical Engineering
Period: 01/08/1996 → 01/08/1999
Number of participants: 1
Project Manager, organisational:
Jakobsen, Sune (Intern)
Project

Ristefyring af biomasse

Department of Chemical and Biochemical Engineering
Period: 01/08/1996 → 06/04/2001
Number of participants: 4
Phd Student:
Røjel, Hanne (Intern)
Supervisor:
Jensen, Anker Degn (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Hansen, Peter F. Binderup (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

Monitoring and Fault Diagnosis
Department of Chemical and Biochemical Engineering
Period: 01/07/1996 → …
Number of participants: 6
Phd Student:
Gregersen, Lars (Intern)
Supervisor:
Jørgensen, Henrik Steen (Ekstern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Thyregod, Poul (Intern)
MacGregor, John F. (Ekstern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Optimization and Control of Biological
Department of Chemical and Biochemical Engineering
Period: 01/07/1996 → 14/03/2002
Number of participants: 5
Phd Student:
Krühne, Ulrich (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Harremoës, Poul (Intern)
Dupont, René (Ekstern)
Olsson, Gustaf (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden Forskningsrådsfinan.-SU
Project: PhD

Automatisk regulering af biologisk spildevandsanlæg
Department of Chemical and Biochemical Engineering
Period: 01/04/1996 → 03/05/2002
Number of participants: 5
Phd Student: Meinhold, Jens (Intern)
Main Supervisor: Jørgensen, Sten Bay (Intern)
Examiner: Henze, Mogens (Intern)
Nielsen, Marinus V. (Ekstern)
von Loosdrecht, Mark (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

**Overgangsmetalkomplekskatalyseret**
Department of Chemical and Biochemical Engineering
Period: 01/04/1996 → 01/10/1998
Number of participants: 2
Phd Student: Rasmussen, Mikael (Intern)
Main Supervisor: Hjortkjær, Jes (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

**Reduktion af Nox fra kalcinatorsystemer**
Department of Chemical and Biochemical Engineering
Period: 01/03/1996 → ...
Number of participants: 5
Phd Student: Jensen, Lars Skaarup (Intern)
Main Supervisor: Glarborg, Peter (Intern)
Examiner: Hansen, Peter F. Binderup (Ekstern)
Livbjerg, Hans (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

**Strukturudvikling i flerfase polymerblanding**
Department of Chemical and Biochemical Engineering
Period: 01/03/1996 → 21/10/1999
Number of participants: 3
Phd Student: Lindquist, Morten (Intern)
Main Supervisor: Lyngaae-Jørgensen, Jørgen (Intern)
Examiner: Hansen, Charles Medom (Ekstern)
**Financing sources**
Source: Internal funding (public)
Name of research programme: Program Stipendium-SU, Eksp
Project: PhD

**Dannelse af organiske faste faser i kulbrinteblandinger**
Department of Chemical and Biochemical Engineering
Period: 01/02/1996 → 23/04/1999
Number of participants: 2
Phd Student:
Lindeloff, Niels (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

**Feilmålunger af forbrændingsaerosoler**
Department of Chemical and Biochemical Engineering
Period: 01/02/1996 → 20/03/2002
Number of participants: 5
Phd Student:
Nielsen, Morten Thellefsen (Intern)
Main Supervisor:
Livbjerg, Hans (Intern)
Examiner:
Johnsson, Jan Erik (Intern)
Christensen, Kurt Agerbæk (Ekstern)
Kauppinen, Esko I. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samarbejdsaftalefinans
Project: PhD

**Membrane - solute interactions in micro**
Department of Chemical and Biochemical Engineering
Period: 01/02/1996 → 21/10/1999
Number of participants: 3
Phd Student:
Thom, Volkmar (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Lyngaae-Jørgensen, Jørgen (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Program Stipendium-SU, Eksp
Project: PhD

**Modellering af stoftransport i membraner**
Department of Chemical and Biochemical Engineering
Period: 01/02/1996 → 01/01/2001
Number of participants: 2
Phd Student:
Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Surface modification of polymeric membranes
Department of Chemical and Biochemical Engineering
Period: 01/02/1996 → 31/01/1999
Number of participants: 2
Project participant:
Thom, Volkmart (Intern)
Project Manager, organisational:
Jonsson, Gunnar Eigil (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner
Project

Control of Biological Waste Water Treatment Plants
Department of Chemical and Biochemical Engineering
Department of Biotechnology
Period: 01/01/1996 → 31/01/1997
Number of participants: 6
Project participant:
Isaacs, Steven Howard (Intern)
Krühne, Ulrich (Intern)
Meinhold, Jens (Intern)
Løfvall, Jan Michael (Intern)
Søeberg, Henrik (Intern)
Project Manager, organisational:
Kymmel, Mogens (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 898,000.00 Danish Kroner
Project

Determination of two-dimensional saturation profiles in cores by nuclear techniques
Department of Automation
Department of Physics
Department of Chemistry
Department of Chemical and Biochemical Engineering
Geological Survey of Denmark and Greenland
Period: 01/01/1996 → 31/12/1996
Number of participants: 3
Project participant:
Korsbech, Uffe C C (Intern)
Ølgaard, Povl Lebeck (Intern)
**Efficient and Clean Use of Biomass for Power and Heat Production. Phase I.**

Pretreatment of biomass fuels for power production. Fluid bed combustion of biomass. Ash formation and emission of trace compounds. Formation and sinting of deposits.

Department of Chemical and Biochemical Engineering

**Project**

**Period:** 01/01/1996 → 31/12/1998

**Number of participants:** 13

**Project participant:**
Andersen, Karin Hedebo (Intern)
Jappe Frandsen, Flemming (Intern)
Hansen, Elisabeth Maria Ter H. (Intern)
Hansen, Jørn (Intern)
Bank, Lars Horsdal (Intern)
Hansen, Lone Aslaug (Intern)
Jensen, Peter Arendt (Intern)
Lin, Weigang (Intern)
Michelsen, Hanne Philbert (Intern)
Wolfe, Thomas (Intern)
Jørgensen, Tina Lillan (Intern)
Johnsson, Jan Erik (Intern)

**Project Manager, organisational:**
Dam-Johansen, Kim (Intern)

**Financing sources**

Source: Unknown
Name of research programme: Ukendt
Amount: 189,000.00 Danish Kroner

**Functional polymers and surfaces**

Functionalization at polymer chain ends in order to initiate further chain growth for synthesizing new block copolymers and modify polymer surfaces in order to alter the surface characteristics by attachment of other polymers either by direct reaction or by admixture of phase separating block copolymers.

Department of Chemical and Biochemical Engineering

**Project**

**Period:** 01/01/1996 → 31/12/1996

**Number of participants:** 1

**Project Manager, organisational:**
Kops, Jørgen (Intern)

**Financing sources**

Source: Unknown
Name of research programme: Ukendt
Amount: 4,100,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 5,500,000.00 Danish Kroner

**Gas Solubility in Acetic Acid**

The aim of the project is to make VLE measurements of mixtures containing acetic acid and gaseous components, in order to improve the production of acetic acid.

Department of Chemical and Biochemical Engineering
Lean Burn Engines - Emission Reduction.

Department of Chemical and Biochemical Engineering
Danish Gas Technology Centre A/S
Period: 01/01/1996 → 30/06/1998
Number of participants: 1
Project Manager, organisational:
Jonasson, Ari Jonas (Intern)

Simulation of flow of polymeric liquids
The project involves development of numerical algorithms for simulation of flow of viscoelastic liquids such as polymer melts and solutions.

Department of Chemical and Biochemical Engineering
Period: 01/01/1996 → …
Number of participants: 1
Project Manager, organisational:
Szabo, Peter (Intern)

Solubility of Gases in Acetic Acid
Department of Chemical and Biochemical Engineering
Period: 01/01/1996 → 16/09/1998
Number of participants: 5
Phd Student:
Jonasson, Ari Jonas (Intern)
Main Supervisor:
Rasmussen, Peter (Intern)
Examiner:
Christiansen, Lars J. (Ekstern)
Mollerup, Jørgen (Intern)
Sørensen, Ansgar (Intern)

Transition Metal Complex Catalyzed Hydroformylation in Biphasic Reaction Media
The industrial hydroformylation of alkenes is one of the most important examples of a homogeneously catalyzed process, implying that reactants, products and catalyst are all dissolved in the same liquid. This homogeneity often leads to separation problems, which may be surmounted by immobilization of the catalytically active complex on a solid support, however often leading to poorer activity and selectivity. A different way to oppose the separation problems might involve
the "immobilization" of the catalyst in a mobile phase, i.e. the catalyst should be made soluble in water, and the catalytic hydroformylation should be accomplished as a biphasic liquid process, with reactants and products in an organic phase and with the catalyst in an aqueous phase, easily separable from the organic phase, so that the catalyst could be quantitatively recycled. This process concept will be tested by kinetic investigation of the alkene hydroformylation catalyzed by water soluble rhodium complexes, prepared by sulfonation of the "non-participative" ligands in the catalytically active complexes. For this purpose we have synthesized 3,4-dimethyl-2,5,6-triphenyl- 1-phosphanorborna-2,5-dien (DMTPPNOR) and initiated kinetic examination of the propene hydroformylation in a plug flow reactor containing a fixed bed of a supported liquid phase catalyst based on Rh-DMTPPNOR. Future work includes sulfonation of DMTPPNOR (leading to NORBOS-Na), and preparation of a supported aqueous phase catalyst, which will also be tested against propene hydroformylation in a fixed bed plug flow reactor.

Department of Chemical and Biochemical Engineering
Period: 01/01/1996 → …
Number of participants: 2
Project participant:
Rasmussen, Mikael (Intern)
Project Manager, organisational:
Hjortkjær, Jes (Intern)

Financing sources
Source: Unknown
Name of research programme: Uendt
Amount: 1,383,909.00 Danish Kroner

Computer Aided Modelling
Department of Chemical and Biochemical Engineering
Period: 01/09/1995 → …
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

Design and Control of Time-Varying Chemical Processes
Department of Chemical and Biochemical Engineering
Period: 01/09/1995 → 13/03/2002
Number of participants: 6
Phd Student:
Pedersen, Kurt (Intern)
Supervisor:
Olsson, Lisbeth (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Poulsen, Niels Kjølstad (Intern)
Brabrand, Henrik (Ekstern)
Hagander, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Generel Model til gruppebidragsbaseret forudsigelse af faseligevægte af komplekse blandinger
Department of Chemical and Biochemical Engineering
Period: 01/09/1995 → 08/12/1998
Number of participants: 3
Phd Student:
Abildskov, Jens (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Elbro, Helle Simon (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Modeling, Analyses and Design of

Department of Chemical and Biochemical Engineering
Period: 01/09/1995 → 19/07/1999
Number of participants: 4
Phd Student:
Tessendorf, Stefan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Cameron, David (Ekstern)
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Aerosoldynamik

Department of Chemical and Biochemical Engineering
Period: 01/08/1995 → 20/04/1999
Number of participants: 3
Phd Student:
Johannessen, Tue (Intern)
Main Supervisor:
Livbjerg, Hans (Intern)
Examiner:
Christensen, Kurt Agerbæk (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Kemiske reaktioners ulineære dynamik - indflydelse på design og opreation

Department of Chemical and Biochemical Engineering
Period: 01/08/1995 → 28/04/2000
Number of participants: 4
Phd Student:
Andersen, Britta Rønde (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Cameron, David (Ekstern)
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD
Termodynamik i kompositionel reservoir simulering
Department of Chemical and Biochemical Engineering
Period: 01/08/1995 → 22/04/1999
Number of participants: 3
Phd Student:
Christensen, Jes Reimer (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Frørup, Mikael Dan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

Modificering og karakterisering af grænseflader i polymer-mineral kompositter
Department of Chemical and Biochemical Engineering
Period: 01/07/1995 → 20/10/1998
Number of participants: 4
Phd Student:
Madsen, Nils Berg (Intern)
Supervisor:
Engell, John Emil (Intern)
Wanheim, Tarras (Intern)
Main Supervisor:
Lyngaae-Jørgensen, Jørgen (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Chromatografisk oprensning af proteiner
Department of Chemical and Biochemical Engineering
Period: 01/06/1995 → 07/01/1999
Number of participants: 4
Phd Student:
Bisgaard-Frantzen, Hans (Intern)
Supervisor:
Staby, Arne (Ekstern)
Main Supervisor:
Mollerup, Jørgen (Intern)
Examiner:
Christensen, Jesper Vinther (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Kandidatstipendium ansat på DT
Project: PhD

Superkritiske Teknikker
Department of Chemical and Biochemical Engineering
Period: 01/06/1995 → 26/05/1999
Number of participants: 4
Phd Student:
Borch-Jensen, Christina (Intern)
Main Supervisor:
Mollerup, Jørgen (Intern)
Examiner:
Bøwadt, Søren (Ekstern)
Fangel, Peder (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Program Stipendium-SU, Eksp
Project: PhD

Bælgningsdannelse ved halmtilsatsfyring
Department of Chemical and Biochemical Engineering
Period: 01/05/1995 → 07/01/1999
Number of participants: 3
Phd Student:
Andersen, Karin Hedebo (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Luxhøj, Fritz (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Materials for district heating tubes
Development and test of models for the heat los in polymer foams.
Department of Chemical and Biochemical Engineering
Abb IC Møller A/S
Period: 01/05/1995 → 30/04/1998
Number of participants: 2
Project participant:
Nielsen, Lars Valentin (Intern)
Project Manager, organisational:
Lyngaae-Jørgensen, Jørgen (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 150,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 463,954.00 Danish Kroner

Struktur og termisk ledningsevne af polymere skummaterialer med lukket cellestruktur
Department of Chemical and Biochemical Engineering
Number of participants: 3
Phd Student:
Nielsen, Lars Valentin (Intern)
Main Supervisor:
Lyngaae-Jørgensen, Jørgen (Intern)
Examiner:
Hassager, Ole (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Chromatografisk oprensing af proteiner
Department of Chemical and Biochemical Engineering
Period: 01/03/1995 → 15/06/1999
Number of participants: 4
Phd Student:
Borgbjerg, Ulrik (Intern)
Main Supervisor:
Mollerup, Jørgen (Intern)
Examiner:
Michelsen, Michael Locht (Intern)
Staby, Arne (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Improving and stabilization of aroma in fermented dairy products
Department of Chemical and Biochemical Engineering
Period: 01/03/1995 → 05/11/1998
Number of participants: 4
Phd Student:
Curic, Mirjana (Intern)
Main Supervisor:
Villadsen, John (Intern)
Examiner:
Hammer, Karin (Intern)
Snoep, Jacob Leendert (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Klæbningens reologi
Department of Chemical and Biochemical Engineering
Period: 01/03/1995 → 10/09/1998
Number of participants: 3
Phd Student:
Christensen, Mia Birch (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Lyngaae-Jørgensen, Jørgen (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Minimering af glycerolproduktion under anaerob vækst af Saccharomyces cerevisiae
Department of Chemical and Biochemical Engineering
Numerisk simulering af varmeovergang i en co-roterende skrabevarmeveksler til levnedsmiddelproduktion

Department of Chemical and Biochemical Engineering
Period: 01/03/1995 → 05/05/1999
Number of participants: 4
PhD Student: Karlson, Torben (Intern)
Supervisor: Adler-Nissen, Jens (Intern)
Main Supervisor: Hassager, Ole (Intern)
Examiner: Sørensen, Ansgar (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Numerisk simulering af viskoelastisk strømning

Department of Chemical and Biochemical Engineering
Period: 01/03/1995 → 31/07/1998
Number of participants: 3
PhD Student: Kolte, Mette Irene (Intern)
Supervisor: Hassager, Ole (Intern)
Examiner: Tvergaard, Viggo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Program Stipendium-SU, Eksp
Project: PhD

Fortrængningsprocesser i Porøse Medier

Department of Chemical and Biochemical Engineering
Period: 01/02/1995 → 15/07/1998
Number of participants: 2
PhD Student: Mogensen, Kristian (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
1. Management of Plant Operation and Control
This overall project aims at developing methods for specifying the tasks at the different levels in the control hierarchy. In particular, methods are considered for representing, i.e. modelling, and analysing the tasks. Supervision at individual levels aims at ensuring consistency of the decisions taken at the different levels. The supervision entails plans, data, models and performance.

Department of Chemical and Biochemical Engineering
Period: 01/01/1995 → …
Number of participants: 1
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

Electrodialytic remediation of soil polluted with heavy metals
Electrodialytic soil remediation is an innovative technique, which has been developing since the beginning of the nineties. An electric current is applied to the contaminated soil, and the pollutants are transported by different mechanisms towards the electrodes. To improve the efficiency of the method this research project is focusing on the electromigration of ionic species: by introducing ion exchange membranes in the process some unfavorable effects may be excluded. The project is carried out in collaboration with A/S Bioteknisk Jordrens

Department of Geology and Geotechnical Engineering
Department of Applied Chemistry
Department of Chemistry
Department of Chemical and Biochemical Engineering
A/S Bioteknisk Jordrens
Period: 01/01/1995 → 31/12/1999
Number of participants: 12
Project participant:
Ottosen, Lisbeth M. (Intern)
Hansen, Henrik K. (Intern)
Karlsmose, Bodil (Intern)
Hansen, Lene (Intern)
Jespersen, Rune Dyre (Intern)
Riberio, Alexandra (Intern)
Dame, Anne Juul (Intern)
Christensen, Iben Verenegren (Intern)
Pettersen, Berit W (Intern)
Bech-Nielsen, Gregers (Intern)
Jonsson, Gunnar Eigil (Intern)

Project Manager, organisational:
Villumsen, Arne (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner

Flame generated nano-particles
The synthesis of material by aerosol routes and based on flame generated particles is studied. The scope include the theoretica and experimental characterization of flame reactors and the deposition of particles to form porous membranes

Department of Chemical and Biochemical Engineering
Period: 01/01/1995 → …
Number of participants: 4
Project participant:
Johannessen, Tue (Intern)
Andersen, Sune Klint (Intern)
Wedel, Stig (Ekstern)
Project Manager, organisational:
Livbjerg, Hans (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,800,000.00 Danish Kroner

Flygtighed af salte ved høje temperaturer
Department of Chemical and Biochemical Engineering
Period: 01/01/1995 → 12/11/1996
Number of participants: 3
Phd Student:
Jensen, Jørgen Peter (Intern)
Main Supervisor:
Rasmussen, Peter (Intern)
Examiner:
Sander, Bo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samarbejdsaftale-Finan-SU
Project: PhD

Software modelling fluid/fluid displacement
Finite element simulation of fluid/fluid displacement in tubes and annuli
Department of Chemical and Biochemical Engineering
Shell
Period: 01/01/1995 → 31/12/1996
Number of participants: 2
Project participant:
Rasmussen, Henrik K. (Intern)
Project Manager, organisational:
Hassager, Ole (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 580,000.00 Danish Kroner

Sugar Transport in Aspergillus oryzae
Department of Chemical and Biochemical Engineering
Period: 01/01/1995 → 02/06/1998
Number of participants: 3
Phd Student:
Schmidt, Karsten (Intern)
Main Supervisor:
Villadsen, John (Intern)
Examiner:
Michelsen, Michael Locht (Intern)

Financing sources
Source: Internal funding (public)
**Undersøgelse af byggeomaterialers sorptionsegenskaber**

Department of Chemical and Biochemical Engineering  
Period: 01/01/1995 → 12/03/2000  
Number of participants: 3  
PhD Student:  
Kjær, Ulla Dorte (Intern)  
Main Supervisor:  
Marcussen, Lis (Intern)  
Examiner:  
Aasbeg-Petersen, Kim (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskerakademiets Samfinansier  
Project: PhD

**Modelling, Design and Analysis of Complex Separation Processes**  
Department of Chemical and Biochemical Engineering  
Number of participants: 4  
PhD Student:  
Cisneros, Eduardo Salvador P. (Intern)  
Main Supervisor:  
Gani, Rafiqul (Intern)  
Examiner:  
Christiansen, Lars J. (Ekstern)  
Villadsen, John (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Anden International Finan-SU  
Project: PhD

**Realtime optimering af et olieraffinaderi**  
Department of Chemical and Biochemical Engineering  
Period: 01/10/1994 → …  
Number of participants: 5  
PhD Student:  
Vahid, Ahedi (Intern)  
Main Supervisor:  
Jørgensen, Sten Bay (Intern)  
Examiner:  
Thyregod, Poul (Intern)  
Andersen, Henrik Weisberg (Ekstern)  
Holst, Jan (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Erhvervsforskerordningen  
Project: PhD

**Computer aided design for proces flowsheets der omfatter elektrolyt - og polymer - systemer**  
Department of Chemical and Biochemical Engineering
Period: 01/09/1994 → 17/03/1998
Number of participants: 4
Phd Student:
Thomsen, Kaj (Intern)
Main Supervisor:
Rasmussen, Peter (Intern)
Examiner:
Ireneo, Kikic (Ekstern)
Sander, Bo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Control design of fed-batch fermentation
Department of Chemical and Biochemical Engineering
Period: 01/09/1994 → …
Number of participants: 3
Phd Student:
Zangirolami, Theresa (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden International Finan-SU
Project: PhD

Design and Simulation of Integrated Biochemical Processes
Department of Chemical and Biochemical Engineering
Period: 01/09/1994 → 20/10/1999
Number of participants: 3
Phd Student:
Bagherpour, Khosrow (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Development of New Adsorbents and Adsorption filters

Department of Chemical and Biochemical Engineering
Universidad de Alicante
Centre National de la Recherche Scientifique
University of Technology
Institute for Sorption and Endocology
St. Petersburg Technological Institute

Institute of Chemistry
Period: 01/09/1994 → …
Number of participants: 7
Project participant:
Rodriguez-Reinoso, F. (Ekstern)
Rouquerol, J. (Ekstern)
Streat, M. (Ekstern)
Strelko, V. (Ekstern)
Ivakhnyuk, G. (Ekstern)
Lupashku, Th. (Ekstern)
Project Manager, organisational:
Marcussen, Lis (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 13,116.00 Danish Kroner

Analyse og dimensionering af ulineære processer

Department of Chemical and Biochemical Engineering
Period: 01/08/1994 → 05/10/1999
Number of participants: 2
Phd Student:
Recke, Bodil (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment

Development of a computer aided system for process simulation model generation

Department of Chemical and Biochemical Engineering
Period: 01/08/1994 → 02/08/1999
Number of participants: 4
Phd Student:
Jensen, Anne Krogh (Intern)
Main Supervisor:
Gani, Rafiquil (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Sørensen, Esben Lauge (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment

Low Nox Burners

Department of Chemical and Biochemical Engineering
Period: 01/08/1994 → 21/01/1998
Number of participants: 4
Phd Student:
Pedersen, Lars Storm (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Bendixen, Knud (Ekstern)
Hupa, Mikko (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Modellering af reservoirfluider ved højt tryk og høj temperatur
Department of Chemical and Biochemical Engineering
Period: 01/08/1994 → 22/03/2000
Number of participants: 2
Phd Student:
Gommesen, Søren (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ef-Finansieret, Stipen.-SU
Project: PhD

Morfologi og proteinsekretion i Aspergillus oryzae
Department of Chemical and Biochemical Engineering
Number of participants: 3
Phd Student:
Spohr, Anders Bendsen (Intern)
Main Supervisor:
Villadsen, John (Intern)
Examiner:
Frisvad, Jens Christian (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Multichannel Reactions and Kinetic Modeling of Combustion Processes
The goal is to provide improved kinetic mechanisms for combustion processes involving complex multichannel reactions. Emphasis is put on aromatics oxidation chemistry.
Department of Chemical and Biochemical Engineering
University of Zaragoza
Period: 01/08/1994 → 01/08/1997
Number of participants: 3
Project participant:
Dam-Johansen, Kim (Intern)
Hansen, Jørn (Intern)
Project Manager, organisational:
Glarborg, Peter (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 300,000.00 Danish Kroner
Project
**Plantwide Control of Generic Integrated Methanol Plant**

Department of Chemical and Biochemical Engineering  
**Period:** 01/08/1994 → 18/09/1998  
**Number of participants:** 2  
Phd Student:  
Hansen, Jens Erik (Intern)  
Main Supervisor:  
Jørgensen, Sten Bay (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Erhvervsforskerordningen  
Project: PhD

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**Aerosoldannelse ved forbrænding af halm**

Department of Chemical and Biochemical Engineering  
**Period:** 01/07/1994 → 18/01/1999  
**Number of participants:** 3  
Phd Student:  
Nielsen, Lars Balzer (Intern)  
Main Supervisor:  
Livbjerg, Hans (Intern)  
Examiner:  
Sander, Bo (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Sektorministerium, Stip-SU  
Project: PhD

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**Danish Polymer Centre**

The research is distributed in 4 main areas: 1) Structure and phase properties of polymer systems. This area is headed by J. Lyngaae-Jørgensen. 2) Polymer rheology and processing. This area is headed by O. Hassager. 3) Functional polymers and surfaces. This area is headed by J. Kops. 4) Liquid crystalline polymers for optical applications.

Department of Chemical and Biochemical Engineering  
Risø National Laboratory  
Coloplast Danmark A/S  
M&E A/S  
Danfoss A/S  
Grundfos A/S  
Nunc A/S  
Hempel A/S  
Novo Nordisk A/S  
Abb IC Møller A/S

**Period:** 01/07/1994 → 30/06/1998  
**Number of participants:** 19  
Project participant:  
Besold, Gerhard (Intern)  
Karlson, Torben (Intern)  
Kolte, Mette Irene (Intern)  
Kops, Jørgen (Intern)  
Lyngaae-Jørgensen, Jørgen (Intern)
Structuring of polymer blends and alloys

Department of Chemical and Biochemical Engineering

Forskningscenter Risø
Period: 01/07/1994 → 01/07/1998
Number of participants: 2
Project participant:
Lindquist, Morten (Intern)
Project Manager, organisational:
Lyngaae-Jørgensen, Jørgen (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 10,600,000.00 Danish Kroner

Et eksperimentelt studium af gashydraters kimdannelse

Department of Chemical and Biochemical Engineering

Period: 01/06/1994 → 09/09/1997
Number of participants: 4
Phd Student:
Bylov, Martin (Intern)
Main Supervisor:
Rasmussen, Peter (Intern)
Examiner:
Mollerup, Jørgen (Intern)
Nerheim, Ann Rigmor (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Electro-Membrane Processes for Flue Gas Cleaning
Department of Chemical and Biochemical Engineering
Period: 01/05/1994 → 29/08/1997
Number of participants: 4
Phd Student:
Larsen, Tommy F. (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Madsen, Rud Frik (Ekstern)
Sander, Bo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

New membrane separation processes
Department of Chemical and Biochemical Engineering

FLS Miljø A/S
Period: 01/05/1994 → …
Number of participants: 3
Project participant:
Rype, Jens-Ulrik (Intern)
Larsen, Tommy F. (Intern)
Project Manager, organisational:
Jonsson, Gunnar Eigil (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner
Project

Uorganiske metalforbindelser i forbrænding og forgasning
Department of Chemical and Biochemical Engineering
Period: 01/04/1994 → 16/03/1999
Number of participants: 4
Phd Student:
Michelsen, Hanne Philbert (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Blum, Hans Jakob R. (Ekstern)
Sander, Bo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Uorganiske metalforbindelser i forbrænding og forgasning
Department of Chemical and Biochemical Engineering
Period: 01/04/1994 → 13/02/1998
Number of participants: 3
Phd Student:
Hansen, Lone Aslaug (Intern)
Main Supervisor:
Fuzzy Based Supervisory Control of Time-varying and Multi-variable Processes

Department of Chemical and Biochemical Engineering
Period: 01/03/1994 → …
Number of participants: 4
Phd Student:
Yazdi, Hassan (Intern)
Supervisor:
Jantzen, Jan (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Kymmel, Mogens (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Center-Finansieret-SU
Project: PhD

1.1 Integration of Supervision and Control
1. Control Structuring for DEDS systems 2. Autonomous DEDS Controller: Supervisory Control Tasks

Department of Chemical and Biochemical Engineering
Period: 01/02/1994 → …
Number of participants: 2
Project participant:
Yazdi, Hassan (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

1.2 Plant Wide Control and Real Time Optimization
1. Design and optimization process plants incl. recycles and heat exchanger networks. 2. Control structuring of integrated plants. 3. Optimizing control of integrated plants. 4. Real Time Optimization

Department of Chemical and Biochemical Engineering
Period: 01/02/1994 → …
Number of participants: 3
Project participant:
Andersen, Torben Ravn (Intern)
Pedersen, Kurt (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

1.3 Process Monitoring, Diagnosis and Optimization

Department of Chemical and Biochemical Engineering
Period: 01/02/1994 → …
Number of participants: 2
Project participant:
Numerisk simulering af strømning af polymere

Department of Chemical and Biochemical Engineering
Period: 01/02/1994 → 31/10/1996
Number of participants: 2
Phd Student:
Nielsen, Michael Almer (Intern)
Main Supervisor:
Hassager, Ole (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Aerosols from the combustion of straw
The size distribution, morphology and chemical composition of aerosols from coal/straw co-combustion are characterized by field measurements on Danish power plants. A theory for the mechanisms of particle formation is developed and tested by laboratory measurements.

Department of Chemical and Biochemical Engineering
Period: 01/01/1994 → …
Number of participants: 3
Project participant:
Nielsen, Lars Balzer (Intern)
Wedel, Stig (Ekstern)
Livbjerg, Hans (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 2,500,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 200,000.00 Danish Kroner
Project

Development of chemical and biological processes for production of bioethanole

Department of Environmental Science and Engineering
Department of Chemical and Biochemical Engineering
Department of Environmental Engineering

RISØ
Period: 01/01/1994 → 01/03/1997
Number of participants: 3
Project participant:
Nørgaard, Claus Schmidt (Intern)
Jensen, Kaj (Intern)
Ahrling, Birgitte Kjaer (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 3,640,000.00 Danish Kroner

**Influence of Process Parameters on Coal Combustion Performance**
Ph.D. project on low NOx pulverized coal combustion, including a cold flow mixing study, coal combustion experiments in different scale plant, and heat transfer modeling of full scale plant.

Department of Chemical and Biochemical Engineering  
Period: 01/12/1993 → 01/05/1997  
Number of participants: 1  
Project Manager, organisational:  
Lans, Robert Pieter Van Der (Intern)

**Models for Pulverized Coal and Fluidized Bed Combustors**

Department of Chemical and Biochemical Engineering  
Period: 01/12/1993 → 11/09/1997  
Number of participants: 4  
PhD Student:  
Lans, Robert Pieter Van Der (Intern)  
Supervisor:  
Glarborg, Peter (Intern)  
Main Supervisor:  
Dam-Johansen, Kim (Intern)  
Examiner:  
Hupa, Mikko (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samarbejdsaftale-Finan-SU  
Project: PhD

**Marine transport of dangerous goods on inland waterways and in coastal areas.**

Department of Chemical and Biochemical Engineering  
Number of participants: 4  
PhD Student:  
Rømer, Hans Gottberg (Intern)  
Supervisor:  
Petersen, H J Styhr (Intern)  
Main Supervisor:  
Kops, Jørgen (Intern)  
Examiner:  
Rasmussen, Birgitte (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Ef-Finansieret, Stipen.-SU  
Project: PhD

**Metaboiske fluxe i Penicillium chrysogenum.**

Department of Chemical and Biochemical Engineering  
Period: 01/08/1993 → 14/01/1997  
Number of participants: 4  
PhD Student:  
Henriksen, Claus Maxel (Intern)  
Supervisor:  
Nielsen, Jens (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Morfologisk karakterisering af penicillium chysogenum.
Department of Chemical and Biochemical Engineering
Period: 01/08/1993 → 23/10/1997
Number of participants: 5
Phd Student: Krabben, Preben (Intern)
Supervisor: Nielsen, Jens (Intern)
Main Supervisor: Villadsen, John (Intern)
Examiner:Christensen, Lars Højlund (Ekstern)
Emborg, Claus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Center-Finansieret-SU
Project: PhD

Low Temperature Nitrogen Chemistry
An experimental and theoretical study of the reburning and advanced reburning processes for nitrogen oxide emission control is undertaken for the 1000-1500 K range.
Department of Chemical and Biochemical Engineering
Danish Gas Technology Centre A/S
Period: 01/07/1993 → 30/06/1996
Number of participants: 3
Project participant: Dam-Johansen, Kim (Intern)
Hansen, Jørn (Intern)
Project Manager, organisational: Glarborg, Peter (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 450,000.00 Danish Kroner
Project

Nye polymermaterialer til optisk informationsbehandling.
Department of Chemical and Biochemical Engineering
Period: 01/06/1993 → 23/07/1997
Number of participants: 3
Phd Student: Strange, Marianne (Intern)
Main Supervisor:
Effective Electrical Conductivity of Porous Beds
Electrostatic filters are widely used for removal of particles from flue gases and other industrial exhaust gases. The electrical conductivity of the porous deposition on the electrodes is a crucial parameter in the design and operation of electrostatic filters since it influences the stability and efficiency of the filters. The purpose of the theoretical and experimental work is to investigate the transport mechanisms in the porous bed, to identify the parameters influencing the effective electrical conductivity, and to derive a mathematical model. An experimental set-up has been constructed and experiments have been and will be performed for a number of parameters. A tentative mathematical model has been derived. It is evaluated and adjusted on the basis of the achieved experimental results.

Adsorptive and chromatographic behaviour of proteins
Measurement and modelling of: Adsorption isotherms Isocratic elution Gradient elution Frontal analysis Mass transfer Properties of proteins in solution

Combustion and Harmful Emission Control
Jensen, Anker Degn (Intern)
Hansen, Jørn (Intern)
Bank, Lars Horsdal (Intern)
Wolfe, Thomas (Intern)
Johnsson, Jan Erik (Intern)
Project Manager, organisational:
Dam-Johansen, Kim (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 10,000,000.00 Danish Kroner

Inorganic Catalysis
Multidisciplinary investigations of structure and catalytic activity of inorganic catalysts and model systems. In collaboration with ICAT.

Department of Chemistry
Department of Physics
Department of Chemical and Biochemical Engineering
University of Patras
Université de Provence
Institute of Catalysis
Georgia Institute of Technology
B.P. Chemicals SA
Haldor Topsoe AS
University of Copenhagen
Period: 01/01/1993 → …
Number of participants: 25
Project participant:
Eriksen, Kim Michael (Intern)
Berg, Rolf W. (Intern)
Holten, Bodil Fliis (Intern)
Nielsen, Kurt (Intern)
Rasmussen, Søren Birk (Intern)
Mattsson, Rikke Christina (Intern)
Barfod, Rasmus (Intern)
Riisager, Anders (Intern)
Boghosian, Soghomon (Ekstern)
Hatem, Gerard (Ekstern)
Gaune-Escard, Marcelle (Ekstern)
Balzhinimaev, Bair (Ekstern)
Lapina, Olga (Ekstern)
Winnick, Jack (Ekstern)
Oehlers, Cord (Ekstern)
Schoubye, Peter (Ekstern)
Topsoe, Nan Yu (Ekstern)
Hyldtoft, Jens (Ekstern)
Thorhauge, Max (Ekstern)
Gabrielson, Per (Ekstern)
Teunissen, Herman (Ekstern)
Møller, Preben Juul (Ekstern)
Spektral element simulering af ultrafiltrering.
Department of Chemical and Biochemical Engineering
Period: 01/01/1993 → 11/09/1996
Number of participants: 5
Phd Student:
Hansen, Michael (Intern)
Supervisor:
Barker, Vincent A. (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Gervang, Bo Groht (Intern)
Madsen, Rud Frik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Development of an improved microwave apparatus for detection of high pressure dew and bubble points
Department of Chemical and Biochemical Engineering
Period: 09/12/1992 → 27/02/1997
Number of participants: 2
Phd Student:
Sendrup, Peter William (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

3.1 Wet-oxidation Reactor
This reactortype is used for oxidation of organic waste production in water at high, but subcritical, pressure at temperatures up to 290 C. The main products are lower organic acids which can be decomposed in a conventional waste water treatment plant. Several aspects including gas phase fraction and pH have been investigated. Lately, an overall oxygen mass transfer coefficient has been estimated from experimental data at a few flow rates.

Department of Chemical and Biochemical Engineering
3. Process Applications

Various aspects of process modelling, design, dynamics and multivariable control are investigated for different process systems. These examples provide both inspiration for significant methodological developments and challenging test grounds for the developed methods.

Department of Chemical and Biochemical Engineering

Period: 01/12/1992 → ...
Number of participants: 1
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

**On-line monitoring of the penicillin fermentation**

Department of Chemical and Biochemical Engineering

Period: 01/12/1992 → 18/12/1995
Number of participants: 2
Phd Student:
Rong, Weimin (Intern)
Main Supervisor:
Villadsen, John (Intern)

**Financing sources**

Source: Internal funding (public)
Name of research programme: Selvfinansierende (privatist)
Project: PhD

**Phase Equilibria in petroleum fluids: multiphase regions and waxformation.**

Department of Chemical and Biochemical Engineering

Period: 01/12/1992 → 23/04/1996
Number of participants: 2
Phd Student:
Coutinho, Joao (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

**Financing sources**

Source: Internal funding (public)
Name of research programme: anden international finansiering
Project: PhD

**Structured models for yeast**

Department of Chemical and Biochemical Engineering

Period: 01/12/1992 → 24/08/1995
Number of participants: 2
Phd Student:
Schulze, Ulrik (Intern)
Main Supervisor:
Villadsen, John (Intern)

**Financing sources**

Source: Internal funding (public)
Name of research programme: Centerfinansiering
Simulering af forbedret olieindvinding (IOR) med avancerede termodynamiske modeller

Department of Chemical and Biochemical Engineering
Period: 01/11/1992 → 27/02/1997
Number of participants: 2
Phd Student: Jørgensen, Marianne (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Nordisk finansiering
Project: PhD

Integrated operational and process-optimization of processes

Department of Chemical and Biochemical Engineering
Period: 01/10/1992 → …
Number of participants: 2
Phd Student: Nielsen, Jan Sandvig (Intern)
Main Supervisor: Jørgensen, Sten Bay (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ATV- Gammel ordning
Project: PhD

Separation process synthesis, design and analysis based on thermodynamic insights.

Department of Chemical and Biochemical Engineering
Period: 01/10/1992 → 23/04/1996
Number of participants: 2
Phd Student: Jaksland, Cecilia (Intern)
Main Supervisor: Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Nordisk finansiering
Project: PhD

Multikomponent adsorption

Department of Chemical and Biochemical Engineering
Number of participants: 3
Phd Student: Krøll, Annette Elisabeth (Intern)
Main Supervisor: Marcussen, Lis (Intern)
Examiner: Aasbeg-Petersen, Kim (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Use of equations of state in compositional reservoir simulation
Ph.D.-project.

Department of Chemical and Biochemical Engineering
Period: 01/08/1992 → 01/09/1996
Number of participants: 1
Project Manager, organisational:
Jørgensen, Marianne (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner

Design og analyse af superkritiske ekstraktionsprocesser.

Department of Chemical and Biochemical Engineering
Period: 01/06/1992 → 18/12/1995
Number of participants: 2
Phd Student:
Hytoft, Glen (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådene via projektbe

Hydrophilt bæremateriale til kemik fastfasesynthese.

Department of Chemical and Biochemical Engineering
Period: 01/06/1992 → 29/06/1995
Number of participants: 2
Phd Student:
Winther, Lars (Intern)
Main Supervisor:
Kops, Jørgen (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier

Rhodiumkomplexkatalysert reduktiv carbonylering af alkoholer

Department of Chemical and Biochemical Engineering
Period: 01/06/1992 → 31/01/1994
Number of participants: 2
Phd Student:
Jensen, Johnny (Intern)
Main Supervisor:
Hjortkjær, Jes (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådene via projektbe

A study of phase equilibria behavior of polydisperse polymer-solvent systems

Department of Chemical and Biochemical Engineering
Period: 01/04/1992 → 18/09/1995
Number of participants: 2
PhD Student:
Goncalves, Ana Saraiva (Intern)
Main Supervisor:
Rasmussen, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Fluid phase equilibria of polymer solutions

Department of Chemical and Biochemical Engineering
Period: 01/04/1992 → 18/04/1995
Number of participants: 2
PhD Student:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Rasmussen, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Aerosoldannelse ved gasfasereaktioner

Department of Chemical and Biochemical Engineering
Period: 01/02/1992 → 12/12/1994
Number of participants: 2
PhD Student:
Christensen, Peter Seier (Intern)
Main Supervisor:
Livbjerg, Hans (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-stipendium
Project: PhD

Flerfasestrømning i annulære tværsnit

Department of Chemical and Biochemical Engineering
Period: 01/02/1992 → 26/08/1994
Number of participants: 3
PhD Student:
Szabo, Peter (Intern)
Main Supervisor:
Hassager, Ole (Intern)
Examiner:
Reffstrup, Jan Otto (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD
**Forstævelighed af viskoelastiske væsker.**

Department of Chemical and Biochemical Engineering  
Period: 01/02/1992 → 29/06/1995  
Number of participants: 3  
Phd Student: Rasmussen, Henrik K. (Intern)  
Main Supervisor: Hassager, Ole (Intern)  
Examiner: Barker, Vincent A. (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-stipendium  
Project: PhD  

**Modelling of growth and product formation in fermentation of filamentous fungi.**

Department of Chemical and Biochemical Engineering  
Period: 01/02/1992 → 31/01/1995  
Number of participants: 2  
Phd Student: Carlsen, Morten (Intern)  
Main Supervisor: Villadsen, John (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-stipendium  
Project: PhD  

**Sporstoffer i forbrændingsprocesser**

Department of Chemical and Biochemical Engineering  
Period: 01/11/1991 → 29/05/1995  
Number of participants: 4  
Phd Student: Jappe Frandsen, Flemming (Intern)  
Supervisor: Larsen, Arne Nylandsted (Ekstern)  
Main Supervisor: Dam-Johansen, Kim (Intern)  
Examiner: Klitgaard, Jørgen (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Gammel ordning u/skema-SU  
Project: PhD  

**Membrane contactor to replace conventional scrubbers**

Department of Chemical and Biochemical Engineering  
Period: 01/10/1991 → 01/01/1995  
Number of participants: 5  
Phd Student: Iversen, Steen Brummerstedt (Intern)  
Supervisor: Barker, Vincent A. (Intern)  

Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Madsen, Rud Frik (Ekstern)
Sander, Bo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ATV- Gammel ordning
Project: PhD

Nitrogenkemi under forbrænding
Department of Chemical and Biochemical Engineering
Period: 01/10/1991 → 18/12/1995
Number of participants: 3
Phd Student:
Kristensen, Per Graves (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Klitgaard, Jørgen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel Ordning - Blandet Finan
Project: PhD

Modellering af vækst og produktdannelse for fermenteringer med penicillium chrysogenum
Department of Chemical and Biochemical Engineering
Period: 01/08/1991 → 16/02/1994
Number of participants: 2
Phd Student:
Johansen, Claus Lindvald (Intern)
Main Supervisor:
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Nitrogen chemistry in fluidized bed combustion
Department of Chemical and Biochemical Engineering
Period: 01/08/1991 → 09/07/1996
Number of participants: 3
Phd Student:
Jensen, Anker Degn (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Klitgaard, Jørgen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-stipendium
Project: PhD
Adsorption/Desorption in Building Materials

Indoor pollutants such as VOCs (Volatile Organic Compounds) are suspected to cause health problems. Adsorption and desorption of VOCs can change and in some cases be decisive for the dynamic spreading and removal of organic compounds in the indoor air. Consequently, the sorption properties of building materials should be considered when planning building operations. This means that the sorption processes and their dependence on the surroundings must be known. Theoretical and experimental work is performed according to this research plan: Lab size experiments for investigation of sorption mechanisms and dynamics for carefully selected building materials and VOCs. In addition, the influence of indoor air temperature, humidity, velocity, VOC concentrations and ozone content is studied. The lab size experiments are tested by means of full scale experiments for the same materials and VOCs. Sensory evaluation of air quality: In addition to the measurement of concentrations during the experiments, it is also planned to perform sensory evaluation of air quality in the test chambers by means of a panel of judges. This supplements the experimentally
determined VOC concentrations, since at present the chemical analysis is not sufficient for prediction of the perceived air quality. Development of mathematical models for the sorption processes and their influence on VOC concentrations in the air. Development of a test method for the characterization of sorption properties of indoor materials.

Department of Chemical and Biochemical Engineering

Statens Byggeforskningsinstitut
Period: 01/02/1991 → …
Number of participants: 3
Project participant:
Kjær, Ulla Dorte (Intern)
Nielsen, Peter Andreas (Ekstern)
Project Manager, organisational:
Marcussen, Lis (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 116,000.00 Danish Kroner

Studies of the phase behavior and physical properties of hydrocarbon fluids

Department of Chemical and Biochemical Engineering
Period: 01/01/1991 → 21/03/1994
Number of participants: 2
Phd Student:
Amin, Robert (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Selvfinansierende (privatist)
Project: PhD

Gas hydrate kinetics

Department of Chemical and Biochemical Engineering
Period: 01/11/1990 → 21/02/1994
Number of participants: 2
Phd Student:
Skovborg, Per (Intern)
Main Supervisor:
Rasmussen, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ATV- Gammel ordning
Project: PhD

Korrelation af gasopløsning og PVT-egenskaber for olie og gas.

Department of Chemical and Biochemical Engineering
Period: 01/11/1990 → 08/01/1996
Number of participants: 2
Phd Student:
Pedersen, Poul Rønning (Intern)
Main Supervisor:
Mollerup, Jørgen (Intern)

Financing sources
Source: Internal funding (public)
Dynamics and control of fixed bed reactors with varying activity

Department of Chemical and Biochemical Engineering
Period: 01/07/1990 → 12/09/1997
Number of participants: 3
Phd Student:
Santiago, Waldemir (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Andersen, Henrik Weisberg (Ekstern)

Financing sources
Source: Internal funding (public)

Application of Membrane Processes in Biotechnology

Department of Chemical and Biochemical Engineering
Period: 01/05/1990 → 18/09/1995
Number of participants: 3
Phd Student:
Wenten, I. Gede (Intern)
Main Supervisor:
Jonsson, Gunnar Eigil (Intern)
Examiner:
Madsen, Rud Frik (Ekstern)

Financing sources
Source: Internal funding (public)

3.5 Periodic Processes

3.5.1 Fixed Bed Reactors, 3.5.2 Periodic Separation

Department of Chemical and Biochemical Engineering
Period: 01/02/1990 → ...
Number of participants: 2
Project participant:
Santiago, Waldemir (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

Gasfasereaktioners afhængighed af ikke ideal strømning

Department of Chemical and Biochemical Engineering
Period: 01/02/1990 → 13/06/1996
Number of participants: 4
Phd Student:
Østberg, Martin (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Hupa, Mikko (Ekstern)
Klitgaard, Jørgen (Ekstern)
**Financing sources**
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

**Biological removal of Phosphorus from wastewater**
Phosphorus can be removed from wastewater either by chemical addition or by biological uptake by specialised bacteria who have such properties that they can be selected for by proper choice of technology. By a sequence of anaerobic and anoxic or aerobic conditions the bacteria are exposed to such condition that they get a favourable situation and will proliferate. In doing so they develop a high intracellular P-content, by which the P is removed from the wastewater with the excess sludge. The aim is to developed a better understanding of the mechanisms of P-uptake and -release in order to better design and control the process in practise.

Department of Environmental Science and Engineering
Department of Chemical and Biochemical Engineering
Period: 01/01/1990 → …
Number of participants: 4
Project participant:
Henze, Mogens (Intern)
Isaacs, Steven Howard (Intern)
Meinhold, Jens (Intern)
Project Manager, organisational:
Harremoës, Poul (Intern)

**Modelling, Identification and control of a continuous fermentation with saccharomyces cerevisiae**
Department of Chemical and Biochemical Engineering
Period: 01/09/1989 → 04/01/1994
Number of participants: 2
Phd Student:
Møller, Hanne Ellen (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)

**Simulering og modelering af termodynamiske data**
Department of Chemical and Biochemical Engineering
Period: 01/09/1989 → 30/05/1994
Number of participants: 2
Phd Student:
Gormsen, Steffen (Intern)
Main Supervisor:
Mollerup, Jørgen (Intern)

**Strukturidentifikation af multivariable kemiske processer**
Department of Chemical and Biochemical Engineering
Period: 01/08/1989 → 27/09/1994
Number of participants: 2
Phd Student:
Rasmussen, Kent Hegnet (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Strømning og sedimentation af suspensioner i komplekse geometrier
Department of Chemical and Biochemical Engineering
Period: 01/10/1988 → 29/06/1995
Number of participants: 2
Phd Student:
Kurtzhals, Erik (Intern)
Main Supervisor:
Hassager, Ole (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Koncentrations- og temperaturmålinger i fyrrum med kulstøvfylding
Department of Chemical and Biochemical Engineering
Number of participants: 3
Phd Student:
Illerup, Jytte Boll (Intern)
Main Supervisor:
Østergaard, Knud (Intern)
Examiner:
Hupa, Mikko (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-stipendium
Project: PhD

Netgenerering
Department of Chemical and Biochemical Engineering
Period: 01/02/1988 → 19/09/1996
Number of participants: 2
Phd Student:
Thomsen, Jan Michael (Intern)
Main Supervisor:
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Supercritical fluid equilibria and chromatography
Phase equilibria of FAEE, fish oil, and other lipids. Analysis of shark oils
Department of Chemical and Biochemical Engineering
FLS Environmental engineering
3.2 Cell Cultivations

Work has been initiated to elucidate cell regulatory mechanisms in a microorganism. These mechanisms play an important role also during relatively short fed-batch cultivations. The ability of this network to adapt to environmental changes may explain the lack of stationarity observed during long continuous cultivations near the optimal operating point.

Department of Chemical and Biochemical Engineering

Novo Nordisk A/S

Technical University of Denmark

Period: 01/01/1987 → ...

Number of participants: 1

Project Manager, organisational:

Jørgensen, Sten Bay (Intern)

The phase behavior of petroleum asphaltene

Investigation of various aspects of asphaltene chemistry and phase behavior including flocculation onset titration, asphaltene precipitation (n-C7) yield at elevated temperatures up to 200°C, emulsion stability, Micellization, chemical characterization as well as modelling aspects of the dissolution and precipitation of asphaltenes using various models.

Department of Chemical and Biochemical Engineering

Period: 01/08/1986 → ...

Number of participants: 1

Project Manager, organisational:

Ivar Andersen, Simon (Intern)

CHEC

CHEC is an acronym for the fundamental and applied research programme on Combustion and Harmful Emission Control. CHEC’s main areas of expertise are industrial high-temperature processes, formation and removal of pollutants, particulate solids (characterisation, reactivity and dynamics). Within these areas the objectives are to educate scientists and engineers, to gain new fundamental information on the subjects, to assist industry and public authorities in the selection, development, design and operation of processes in order to improve efficiencies and in order to avoid or minimise harmful emissions, to catalyse international cooperation between Danish companies and Danish and foreign research organisations.

Department of Chemical and Biochemical Engineering

Department of Applied Chemistry

Department of Energy Engineering
University of Zaragoza
Danish Maritime Institute
Danish Gas Technology Centre A/S
GasResearch Institute
Danish Technological Institute
Elsam A/S
Elkraft A.m.b.A.
ELTRA I/S
Faxe Kalk A/S
FLS Miljø A/S
F.L. Smidth A/S
FORCE Institute
Haldor Topsoe AS
Hempel A/S
Niro A/S
Rockwool International
Advanced Fuel Research Inc.
Chalmers University of Technology
International Flame Research Foundation
Mitsui Babcock Energy Ltd
National Risk Management Research Laboratory
Norwegian University of Science and Technology
Nagoya University
Sandia National Laboratories
Hamburg University of Technology
University of Connecticut
University of North Dakota
University of Queensland
University of Stuttgart
VVT Chemical Technology
Åbo Academy University

Period: 10/01/1986 → …
Number of participants: 35
Project participant:
Ambrosius, Margit (Intern)
Bank, Lars Horsdal (Intern)
Becerra, Signe V.r.v. (Intern)
Cenni, Roberta (Intern)
Jappe Frandsen, Flemming (Intern)
Frandsen, Jan (Intern)
Giarborg, Peter (Intern)
Hansen, Elisabeth Maria Ter H. (Intern)
Hansen, Jern (Intern)
Adsorption

TYPICAL APPLICATIONS OF ADSORPTION
Removal of pollutants from gases and liquids, recovery of chemicals, separation of mixtures. MULTICOMPONENT ADSORPTION
Mathematical modelling and experiments: Equilibria and kinetics in ideal and non-ideal multicomponent systems, heat and mass transfer in adsorption processes. INDUSTRIAL ADSORBERS

Department of Chemical and Biochemical Engineering

Project participant:

Krøll, Annette Elisabeth (Intern)

Project Manager, organisational:

Marcussen, Lis (Intern)

Financing sources

Source: Unknown

Name of research programme: Ukendt

Amount: 1,155,000.00 Danish Kroner

Source: Unknown

Name of research programme: Ukendt

Amount: 13,956.00 Danish Kroner
3.3 Distillation
a. Validation of simulation and simplified dynamic model b. Control structure determination c. Identification for multivariable control d. Optimizing control e. Multiplicity and stability in distillation f. Homogen azeotrop distillation g. Heterogen azeotrop distillation h. Reactive distillation Experiments have been conducted aiming at verifying the existence of input multiplicities within an optimal operating region. One multiplicity presumably caused by tray efficiency variations have been demonstrated.

Department of Chemical and Biochemical Engineering
Period: 01/02/1982 → …
Number of participants: 3
Project participant:
Andersen, Torben Ravn (Intern)
Yazdi, Hassan (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

Simulation of phase equilibrium and separation processes
The purpose of the project, which is conducted within the IVC-SEP centre, is to develop efficient and robust algorithms for the simulation of phase equilibrium and separation processes. The project also deals with the development and implementation of models for calculation of phase equilibrium and the development of computational tools for this purpose. Algorithms from the Institute are today used worldwide, in particular in the petroleum industry. Recent efforts are concentrated on complex equilibria, as e.g. the treatment of 3-phase equilibria in oil mixtures containing water and hydrate inhibitors, and on developing procedures for cases where the computational speed is all-important, such as flow- and reservoir simulators.

Department of Chemical and Biochemical Engineering
Center for Energy Resources Engineering
Period: 01/01/1980 → 01/01/1981
Number of participants: 1
Project Manager, organisational:
Michelsen, Michael Locht (Intern)

2.1 Reactor Dynamics

Department of Chemical and Biochemical Engineering
Period: 01/07/1972 → …
Number of participants: 3
Project participant:
Recke, Bodil (Intern)
Andersen, Britta Rønde (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

2.2 Design and Control of Safety Critical Processes
1. Design and operation margins for safety critical reactions. 2. Possible benefits from control.

Department of Chemical and Biochemical Engineering
Period: 01/07/1972 → …
Number of participants: 2
Project participant:
Recke, Bodil (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)
2.3 Multivariable Process Identification for Control
This project aims at using knowledge on process and disturbance dynamics to structure relatively low order models which subsequently are experimentally identified together with an uncertainty description which is related to the assumed disturbances.

Department of Chemical and Biochemical Engineering
Period: 01/07/1972 → …
Number of participants: 1
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

2. Chemical Process Dynamics and Control
Most process plants are driven to operate near their optimal operating region where nonlinear behaviour may seriously affect the dynamic behaviour. The purposes of this project are to elucidate possible behaviours and to investigate the possibility for preventing undesirable behaviour through modified process or control design.

Department of Chemical and Biochemical Engineering
Period: 01/07/1972 → …
Number of participants: 1
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

3.4 Fixed Bed Reactor
1. Dynamics with unconverted reactant recycling 2. Control near critical points. Experimental work has been initiated to attempt to reveal existence of some typical bifurcation behaviours.

Department of Chemical and Biochemical Engineering
Period: 01/07/1972 → …
Number of participants: 2
Project participant:
Recke, Bodil (Intern)
Project Manager, organisational:
Jørgensen, Sten Bay (Intern)

Membrane Filtration
Investigations of solvent and solute transport for the membrane processes reverse osmosis, nanofiltration, ultrafiltration and microfiltration.

Department of Chemical and Biochemical Engineering
Period: 01/03/1970 → …
Number of participants: 4
Project participant:
Guerra, Marie Alexandra (Intern)
Jakobsen, Sune (Intern)
Garde, Arvid (Intern)
Project Manager, organisational:
Jonsson, Gunnar Eigil (Intern)

Thermodynamics of fluids and fluid mixtures
Corresponding states models Equation of state models Models for excess Gibbs energies and equations of state. Properties of proteins in solution Adsorption isotherms

Department of Chemical and Biochemical Engineering
Period: 01/01/1970 → 01/04/2012
Number of participants: 1
Project Manager, organisational:
Mollerup, Jørgen (Intern)
Activities:

Production of alkali from cocoa husk ash and biological extraction of hydrocolloid from Sargassum sp.
Period: 2017
Marcel Tutor Ale (Other)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Description
Coordinated by Marcel Tutor Ale
Activity: Other

Production of alkali from cocoa husk ash for extraction of hydrocolloid from biologically pretreated red seaweed
Period: 2017
Marcel Tutor Ale (Other)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Description
Coordinated by Marcel Tutor Ale
Activity: Other

Model-based optimization of a full-scale industrial anaerobic reactor producing biogas
Period: 10 Dec 2017 → 13 Dec 2017
Hannah Feldman (Speaker)
Xavier Flores Alsina (Other)
Pedram Ramin (Other)
Kasper Kjellberg (Other)
Ulf Jeppsson (Other)
Krist V. Gernaey (Other)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
Degree of recognition: International
Related event
8th International Young Water Professionals Conference
10/12/2017 → 13/12/2017
Cape Town, South Africa
Activity: Talks and presentations › Conference presentations

Wood stove combustion
Period: 23 Nov 2017
Jytte Boll Illerup (Lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
Degree of recognition: National
Documents:
Annual Day 2017 Wood stove combustion_Jytte Illerup
Related event
CHEC Annual Day 2017
23/11/2017 → 23/11/2017
Emulsion Formation for EOR Applications
Period: 14 Nov 2017 → 15 Nov 2017
Muhammad Waseem Arshad (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Center for Energy Resources Engineering

Description
DHRTC Technology Conference 2017
14-15 November, Kolding, Denmark
Documents:
Final-Programme

Related external organisation
Danish Hydrocarbon Research and Technology Centre
Denmark

Real-time monitoring of a fermentation process: linking yeast morphology to insulin production by image analysis
Period: 1 Nov 2017
Katrin Pontius (Guest lecturer)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
PILOT PLANT

Description
Fermentation production processes are often the most complex step within bio-manufacturing. Nevertheless, due to a highly challenging environment inside the bioreactor, industrial fermentation processes are presently rather limited regarding analytical tools for process control. There is a deficit in suitable monitoring devices that can cope with the complexity of the dynamic fermentation environment without compromising the integral success of the process. Therefore, we want to take advantage of the recent advances in microscopy image analysis and evaluate its potential for on-/at-line monitoring of yeast physiology. In yeast cultures, cell size (distribution) has been shown to be correlated with cell viability (dead/alive, osmotically stressed) and growth rate. Furthermore, the cell size was recently correlated to the accumulation of an internal product (fatty acids) in microalgae. Consequently, image analysis seems to be a promising tool for getting a snapshot of the physiological state of a yeast culture during a production process. The lately developed oCelloScope instrument enables rapid imaging and image analysis of a growing yeast culture. By analyzing images over the cultivation time we investigate the distribution dynamics of single cells, budding cells and cell aggregates, aiming at correlations between morphological features and process performance. Ideally, we want to develop a real-time monitoring tool that may be used in industrial bioprocess setups. Within this approach, methodologies for automatic distinction between image objects (single cells, budding cells, cell aggregates) are developed and first time trends of the morphology dynamics of an insulin production process are discussed. 1.Tibayrenc, P., Preziosi-Bello, L., Roger, J. M. & Ghommidh, C. Assessing yeast viability from cell size measurements? J. Biotechnol. (2010). doi:10.1016/j.jbiotec.2010.06.019 2.Caminsard, V., Brienne, J. P., Baussart, H., Hammann, J. & Suhr, H. Inline characterization of cell concentration and cell volume in agitated bioreactors using in situ microscopy: Application to volume variation induced by osmotic stress. Biotechnol. Bioeng. (2002). doi:10.1002/bit.10178 3.Tyson, C. B., Lord, P. G. & Wheals, A. E. Dependency of Size of Saccharomyces cerevisiae Cells on Growth Rate. J. Bacteriol. 138, 92–98 (1979). 4.Marbà-Ardébol, A.-M., Emmerich, J., Neubauer, P. & Junne, S. Single-cell-based monitoring of fatty acid accumulation in Cryptothecodinium cohnii with three-dimensional holographic and in situ microscopy. Process Biochem. 52, 223–232 (2017). 5.Fredborg, M. et al. Real-time optical antimicrobial susceptibility testing. J. Clin. Microbiol. 51, 2047–2053 (2013).
CFD application as a tool for designing industrial fermenters
Period: 29 Oct 2017 → 1 Nov 2017
Ines Pereira Rosinha Grundtvig (Speaker)
Krist V. Gernaey (Other)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
Degree of recognition: International
Documents:
Abstract - Ines Grundtvig

Related event

Recent Advances in Fermentation Technology
29/10/2017 → 01/11/2017
Activity: Talks and presentations › Conference presentations

Dynamics of physiological adaptation of Saccharomyces cerevisiae to biomass hydrolysates: a single cell analysis approach.
Period: 29 Oct 2017 → 2 Nov 2017
Pau Cabañeros Lopez (Other)
Chuen Tao Peng (Other)
Nils Arneborg (Other)
Anna Eliasson Lantz (Other)
Krist V. Gernaey (Other)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
PILOT PLANT
Degree of recognition: International

Related event

Recent Advances in Fermentation Technology (RAFT 2017)
29/10/2017 → 01/11/2017
Florida, United States
Activity: Talks and presentations › Conference presentations

Strategy for characterizing microbial physiology across scales in fermentation processes
Period: 29 Oct 2017
Gisela Nadal Rey (Other)
Sjef Cornelissen (Other)
Anna Eliasson Lantz (Other)
Krist V. Gernaey (Other)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
PILOT PLANT
Description
Poster presentation at RAFT 2017.
Degree of recognition: International

Related event

Recent Advances in Fermentation Technology (RAFT 2017)
29/10/2017 → 01/11/2017
Florida, United States
Modelling Illicit Drug Fate in Sewers for Wastewater-Based Epidemiology
Period: 26 Oct 2017 → 27 Oct 2017
Pedram Ramin (Speaker)
Peter Steen Mikkelsen (Guest lecturer)
Benedek G. Plósz (Guest lecturer)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
Department of Environmental Engineering
Urban Water Systems
Degree of recognition: International
Links:

Related organisation
Modelling Illicit Drug Fate in Sewers for Wastewater-Based Epidemiology
Ramin, P. (Speaker), Mikkelsen, P. S. (Guest lecturer), Plósz, B. G. (Guest lecturer)
26 Oct 2017 → 27 Oct 2017
Activity: Talks and presentations › Conference presentations

Calibration and Validation of an Anaerobic Digestion Model for Process Optimization of an Industrial Granular Sludge Reactor
Hannah Feldman (Speaker)
Xavier Flores Alsina (Other)
Pedram Ramin (Other)
Kasper Kjellberg (Other)
Ulf Jeppsson (Guest lecturer)
Damien J. Batstone (Guest lecturer)
Krist V. Gernaey (Guest lecturer)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
Degree of recognition: International

Related event
The 15th IWA World Conference on Anaerobic Digestion
17/10/2017 → 20/10/2017
Beijing, China
Activity: Talks and presentations › Conference presentations

Surface characterization of activated chalcopyrite particles via the FLSmidth ROL process. Part 2: Surface spectroscopy investigations
Period: 12 Oct 2017
Adam Paul Karcz (Guest lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
Due to its semiconductor properties, the world's most abundant copper mineral, chalcopyrite (CuFeS₂), is refractory with respect to atmospheric leaching using traditional acidic ferric sulfate lixiviants. FLSmidth® has developed a novel Rapid Oxidative Leach (ROL) process that (a) manipulates the lattice and (b) mechano-chemically processes chalcopyrite with a Stirred Media Reactor (SMR). This combination yields the benefit of increasing chemical reactivity and dissolution kinetics. By reducing surface passivation, this process is typically able to achieve copper recoveries exceeding 95% in under 6-8 hours. An important factor contributing to this extraordinary performance is a
mineral preconditioning step, which uses 0.1-5 mol% of copper(II) to dope the lattice and thereby “activate” chalcopyrite. Previously, we reported the relationship between doping and deformation of the chalcopyrite lattice using electron microscopy. Now, we draw further insights into the electrochemical properties of the activated chalcopyrite particles through a variety of surface spectroscopy studies.

Degree of recognition: International

Related event

Materials Science and Technology 2017
08/10/2017 → 12/10/2017
Pittsburgh, United States
Activity: Talks and presentations › Conference presentations

Camera Measurements in Cement Kilns – Impact of Alternative Fuels on Klin Flames
Period: 10 Oct 2017 → 11 Oct 2017
Morten Nedergaard Pedersen (Guest lecturer)
Mads Nielsen (Guest lecturer)
Sønnik Clausen (Guest lecturer)
Peter Arendt Jensen (Guest lecturer)
Lars Skaarup Jensen (Guest lecturer)
Kim Dam-Johansen (Guest lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
The Hempel Foundation Coatings Science and Technology Centre (CoaST)

Description
Presentation and extended abstract given at Nordic Flame Days 2017
Documents:
Extended Abstract Nordic Flame Days 2017 - Morten Pedersen - v2

Related event

Nordic Flame Days
10/10/2017 → 11/10/2017
Stockholm, Sweden
Activity: Talks and presentations › Conference presentations

Combustion of Thermoplastic Particles in Single Particle Combustor
Period: 10 Oct 2017 → 11 Oct 2017
Mohammadhadi Nakhaei (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
Degree of recognition: International
Documents:
Session 1B, MH Nakhaei-NFD2017-11Oct2017

Related event

Nordic Flame Days
10/10/2017 → 11/10/2017
Stockholm, Sweden
Activity: Talks and presentations › Conference presentations

Pelletization of torrefied biomass: a modelling approach
Period: 10 Oct 2017
Maria Puig Arnavat (Speaker)
Marvin Masche (Speaker)
Jesper Ahrenfeldt (Speaker)
Ulrik Birk Henriksen (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

**Description**
The present study aims to apply and validate a simple model for biomass pelletization to describe the pelletization process of wet and dry torrefied biomass (giant reed and willow, respectively). The goal is to allow for a fast estimation of important pelletization parameters by combining a theoretical background with the use of a single pellet press. For this reason, pelletization tests at different die temperatures and compression ratios were carried out and the model was applied to explain the experimental data obtained. The model proved to be a good tool to better understand and describe the pelletizing behaviour of torrefied biomass material.

**Degree of recognition:** International

**Documents:**
Pelletization torrefied biomass - Maria Puig - Extended abstract

**Related event**

**Nordic Flame Days**
10/10/2017 → 11/10/2017
Stockholm, Sweden

Activity: Talks and presentations › Conference presentations

**Operational monitoring of phosphate and ammonium for an industrial fermentation process using infrared (IR) and near-infrared (NIR) spectroscopy**

**Period:** 5 Oct 2017

Katrin Pontius (Speaker)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre

**PILOT PLANT**

**Description**
In the context of protein production via fermentation processes, proteases produced by Bacillus species are a billion dollar business and set nearly 60 % of the global enzyme market. Manufacturers continuously search for new and improved proteases to meet stability and performance demands and robust production processes are important for economically viable production. Thereby, developing robust and generic on-line monitoring techniques is important to meet the need for monitoring and controlling the process at optimal conditions. Phosphorus and ammonium are central nutrients in media for Bacillus fermentations and need to be present in relevant levels to promote growth and enzyme production. Besides, both species impose additional costs on downstream wastewater treatment if more is added to the medium during the fermentation than needed by the microorganism. Hence, there are also major challenges associated with phosphate and ammonium. Note that, fermentation processes usually operate under mild conditions and the products are rather diluted. Therefore, a large amount of wastewater containing nutrients is generated that needs to be treated. On-line monitoring of phosphate and ammonium during fermentation processes would facilitate development of feeding strategies of phosphate and ammonium during protein production ensuring that the nutrients are kept at the correct level. On-line monitoring tools would also provide a better understanding of bioprocess dynamics over the entire line from upstream to downstream.

In this work, a case study focusing on the determination of concentration of phosphate and ammonium in a Bacillus protein production process is considered. Both IR and NIR in combination with partial least square regression (PLS) are being employed in this work. This combined approach provides the means for measuring phosphate and ammonium concentrations in a semi-defined culture medium through real-time/on-line monitoring. The present approach is applied on a lab-scale fermentation setup adjusting the operating conditions to mimic the real operation for an industrial application. To minimize the complexity associated with spectroscopy measurements on fermentation broth and decouple natural correlations of parameters, synthetic samples spiked with phosphate or ammonium in addition to real fermentation samples where applied in the model development process. Thereby, regions of IR and NIR spectra corresponding to phosphate and ammonium were appropriately identified and selected. One major advantage associated with this approach is its selectivity due to the appropriateness of the selection criteria (different wavelengths as variables) that are uniquely tied to the target species. Another advantage lies within the versatility of the (N)IR probe itself that can be used in various bioprocess settings. This generic method development strategy will be presented. Furthermore, the application of the on-line monitoring strategies for phosphate and ammonium during a fed-batch, protein production process will be discussed.

**Related event**
Deactivation of a Cu-CHA NH3-SCR Catalyst by SO2 and SO3
Period: 4 Oct 2017
Peter Sams Hammershøi (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

2017 CLEERS Workshop
03/10/2017 → 05/10/2017
Activity: Talks and presentations › Conference presentations

Advanced fabrication of porous ceramic multilayers for membrane applications
Period: 2 Oct 2017
Andreas Kaiser (Keynote speaker)
Wenjing (Angela) Zhang (Invited speaker)
Manuel Pinelo (Invited speaker)
Michela Della Negra (Other)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Proton conductors
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Degree of recognition: International
Documents:
Icm 2017 - abstract - Andreas Kaiser

Application of a computer-aided framework for the design of CO2 capture and utilization processes
Period: 2 Oct 2017
Rebecca Frauzem (Speaker)
Department of Chemical and Biochemical Engineering
KT Consortium
Description
A presentation of the PhD work being carried out at DTU.
Degree of recognition: International
Related event
27th European Symposium on Computer Aided Process Engineering
01/10/2017 → 05/10/2017
Barcelona, Spain
Activity: Talks and presentations › Conference presentations
Design of a gas-inducing impeller using Computational Fluid Dynamics
Period: 1 Oct 2017 → 5 Oct 2017
Ines Pereira Rosinha Grundtvig (Guest lecturer)
Tim Hybschmann (Other)
Krist V. Gernaey (Other)
Tore C. Svendsen (Other)
Ulrich Krühne (Other)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
Degree of recognition: International
Documents:
Abstract_WCCE_Ines_Grundtvig_2

Related event
10th World Congress of Chemical Engineering (WCCE10)
01/10/2017 → 05/10/2017
Barcelona, Spain
Activity: Talks and presentations › Conference presentations

Topology optimization as a tool for designing microbioreactors
Period: 1 Oct 2017 → 5 Oct 2017
Ines Pereira Rosinha Grundtvig (Speaker)
Anders Egede Daugaard (Other)
John Woodley (Other)
Ulrich Krühne (Other)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
The Danish Polymer Centre
Degree of recognition: International
Documents:
Abstract_WCCE_Ines_Grundtvig_1

Related event
10th World Congress of Chemical Engineering (WCCE10)
01/10/2017 → 05/10/2017
Barcelona, Spain
Activity: Talks and presentations › Conference presentations

10th World Congress of Chemical Engineering (WCCE10)
Period: 29 Sep 2017 → 2 Oct 2017
Rebecca Frauzem (Organizer)
Department of Chemical and Biochemical Engineering
KT Consortium
Description
Part of the Student Conference organizing committee with other students and faculty from universities around the world.
The student conference had a ChemE Car competition, trips to industrial sites, visits to the EXPOQUIMIA and
presentation and discussions for undergraduate and graduate students.
Degree of recognition: International

Related event
10th World Congress of Chemical Engineering (WCCE10)
01/10/2017 → 05/10/2017
Barcelona, Spain  
Activity: Attending an event › Participating in or organising a conference

**TCbiomass 2017**  
Period: 19 Sep 2017 → 21 Sep 2017  
Magnus Zingler Stummann (Participant)  
Department of Chemical and Biochemical Engineering

**Related event**

**TCbiomass 2017: The Global Future of Bioenergy**  
19/09/2017 → 21/09/2017  
Chicago, United States  
Activity: Attending an event › Participating in or organising a conference

**Influence of Promotor, H2O and H2S on the Hydrodeoxygenation of Biomass Pyrolysis Vapor over MoS2 Catalysts**  
Period: Aug 2017  
Trine Marie Hartmann Dabros (Guest lecturer)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre  
**Description**  
Oral presentation  
Documents:  
EuropaCat2017_TrineArndal_Abstract  
**Related event**

**13th European Congress on Catalysis (EUROPACAT 2017)**  
27/08/2017 → 31/08/2017  
Florence, Italy  
Activity: Talks and presentations › Conference presentations  
**Poster Presentation: "Pre-turbo SCR catalyst for NOx removal on Ships"**  
Period: 27 Aug 2017 → 31 Aug 2017  
Steen Müller Christensen (Guest lecturer)  
Brian Brun Hansen (Guest lecturer)  
Keld Johansen (Guest lecturer)  
Anker Degn Jensen (Guest lecturer)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre  
Documents:  
Abstract  
**Related event**

**13th European Congress on Catalysis (EUROPACAT 2017)**  
27/08/2017 → 31/08/2017  
Florence, Italy  
Activity: Talks and presentations › Conference presentations  
**Density-Functional Theory and Beyond**  
Period: 31 Jul 2017 → 12 Aug 2017  
Adam Paul Karcz (Participant)  
Max Schumann (Participant)  
Department of Chemical and Biochemical Engineering
Description
The discovery of novel materials is key on the route to face global challenges like quest for efficient and sustainable use of energy resources. Computational approaches play a central role here as they allow us to explore uncharted territory in chemical and materials space, for example in order to develop novel batteries, highly efficient solar cells, stable biocatalysts, or carbon dioxide fixation strategies.

Novel Materials Discovery by Learning from Electronic-Structure Theory is going to be a central theme of this summer school, we will educate young scientists in the basics and recent advances of electronic-structure theory. The focus will be in particular on density-functional theory (DFT), but also topics beyond DFT will be covered: ab initio thermodynamics and statistical mechanics, excited-state properties, nuclear quantum effects, multi-scale modeling, and machine learning approaches to potential parametrization, Big-Data dimensionality reduction, and property prediction. Such methods are widely applicable from biophysics to materials science and are a driving force for the discovery and design of molecules and materials. During this event, we will discuss the underlying concepts and thereby raise awareness for success stories, problems, and current challenges.

The workshop features morning lectures that introduce basics and advanced topics. In the afternoons, participants will gain experience in hands-on sessions guided by skilled tutors. The main computational workhorse for the afternoon sessions will be the FHI-aims all-electron code, which embodies all necessary methods. The overall workshop, however, is not designed to teach a single code, but rather to introduce scientific concepts.

Degree of recognition: International

Related event

Density-Functional Theory and Beyond: Accuracy, Efficiency and Reproducibility in Computational Materials Science
31/07/2017 → 12/08/2017
Berlin, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Influence of Promotor, H2O and H2S on the Hydrodeoxygenation of Biomass Pyrolysis Vapor over MoS2 Catalysts
Period: Jun 2017
Trine Marie Hartmann Dabros (Guest lecturer)
Anker Degr Jensen (Guest lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
Oral presentation
Documents:
Nam25_TrineArndal_Abstract

Related event

25th North American Catalysis Society Meeting
04/06/2017 → 09/06/2017
Denver, United States
Activity: Talks and presentations › Conference presentations

Solvolyis of Lignosulfonate Catalyzed by Supported NiMo
Period: Jun 2017
Soheila Ghafarnejad Parto (Speaker)
Jakob Munkholt Christensen (Other)
Lars Saaby Pedersen (Other)
Esben Taarning (Other)
Freddy Tjosås (Other)
Anker Degr Jensen (Other)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
Degree of recognition: International
Documents:
Soheila Parto-Abstract

Related event

**21st Annual Green Chemistry and Engineering Conference**  
13/06/2017 → 15/06/2017  
Reston, United States  
Activity: Talks and presentations › Conference presentations

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13th Coating Science International 2017  
Period: 26 Jun 2017 → 30 Jun 2017  
Ting Wang (Participant)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre

**Description**  
13th Coatings Science International 2017  
Degree of recognition: International

Related event

13th Coating Science International 2017  
26/06/2017 → 30/06/2017  
Noordwijk, Netherlands  
Activity: Attending an event › Participating in or organising a conference

**Drag resistance measurements for newly applied antifouling coatings and welding seams on ship hull surface**  
Period: 26 Jun 2017 → 30 Jun 2017  
Xueting Wang (Guest lecturer)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre  
The Hempel Foundation Coatings Science and Technology Centre (CoaST)  
Degree of recognition: International

Related event

13th Coatings Science International Conference 2017  
26/06/2017 → 30/06/2017  
Noordwijk, Netherlands  
Activity: Talks and presentations › Conference presentations

**Quantitative analysis of pigment dispersion taking into account the full agglomerate size distribution**  
Period: 26 Jun 2017 → 30 Jun 2017  
Søren Kiil (Lecturer)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre  
The Hempel Foundation Coatings Science and Technology Centre (CoaST)  
Degree of recognition: International  
Documents:  
Abstract COSI 2017 (Søren Kiil)

Related organisation

Quantitative analysis of pigment dispersion taking into account the full agglomerate size distribution  
Kiil, S. (Lecturer)  
26 Jun 2017 → 30 Jun 2017  
Activity: Talks and presentations › Conference presentations
Tar Removal from Biomass Producer Gas by Using Biochar
Period: 13 Jun 2017
Giulia Ravenni (Guest lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
Oral presentation
Degree of recognition: International
Documents:
2BO.14.2_presentation_25th_2017

Related event
25th European Biomass Conference and Exhibition
12/06/2017 → 15/06/2017
Stockholm, Sweden
Activity: Talks and presentations › Conference presentations

Deactivation of a Cu-SSZ-13 NH₃-SCR Catalyst by SO₂ and SO₃
Period: 8 Jun 2017
Peter Sams Hammershøi (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Related event
North American Catalysis Society Meeting 2017
04/06/2017 → 09/06/2017
Denver, United States
Activity: Talks and presentations › Conference presentations

A new association scheme for mono-ethylene glycol within Cubic-Plus-Association equation of state
Period: 19 May 2017
Francois Kruger (Guest lecturer)
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering

Description
Presentation and poster detailing work on newly proposed association schemes for MEG, along with uncertainty analysis for the parameterization
Degree of recognition: International
Documents:
ESAT 2017: Uncertainty Analysis for the Parameterization of Glycols

Related event
29th European Symposium on Applied Thermodynamics
18/05/2017 → 21/05/2017
Bucharest, Romania
Activity: Talks and presentations › Conference presentations

Feasibility test of a complete autotrophic nitrogen removal process treating the effluent of an industrial anaerobic digester
Period: 9 May 2017 → 12 May 2017
Hannah Feldman (Other)
Modelling Methane, Sulphide and Multiple Mineral Precipitation in a Full-Scale Industrial Granular Anaerobic Digester

Period: 9 May 2017 → 12 May 2017

Hannah Feldman (Other)
Xavier Flores Alsina (Other)
Kasper Kjellberg (Other)
Gürkan Sin (Other)
Krist V. Gernaey (Other)

Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre

Related event
10th International Conference on Biofilm Reactors
09/05/2017 → 12/05/2017
Dublin, Ireland
Activity: Talks and presentations › Conference presentations

Surface properties and chemistry correlate to the digestibility of biomass following hydrothermal pretreatment at different severities

Period: 1 May 2017 → 4 May 2017

Demi Tristan Djajadi (Guest lecturer)
Aleksander R. Hansen (Guest lecturer)
Anders Jensen (Guest lecturer)
Lisbeth G. Thygesen (Guest lecturer)
Manuel Pinelo (Guest lecturer)
Anne S. Meyer (Guest lecturer)
Henning Jørgensen (Guest lecturer)

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Description
Poster presentation
Degree of recognition: International

Related event
39th Symposium on Biotechnology for Fuels and Chemicals
01/05/2017 → 04/05/2017
San Francisco, United States
Activity: Talks and presentations › Conference presentations

**Microbial multi modular xylanolytic enzymes in mesophilic anaerobic digesters fed with wastewater treatment sludge**
Period: 21 Apr 2017
Casper Wilkens (Invited speaker)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Degree of recognition: International

**Related event**
**Satellite Meeting of CBM12**
20/04/2017 → 21/04/2017
Kongens Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Student Info Meeting**
Period: 2016
Marcel Tutor Ale (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

**Description**
Student Info Meeting

**Related event**
**Student Info Meeting**
01/01/2016 → 01/01/2016
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Safeprops: A Software for Fast and Reliable Estimation of Safety and Environmental Properties for Organic Compounds**
Period: 16 Nov 2016
Mark Nicholas Jones (Lecturer)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Links:
https://aiche.confex.com/aiche/2016/webprogram/Paper466860.html

**Related external organisation**
**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**2016 AIChE Annual Meeting**
Period: 13 Nov 2016 → 18 Nov 2016
Rebecca Frauzem (Speaker)
Department of Chemical and Biochemical Engineering
KT Consortium

**Description**
I gave 2 presentations and participated in the remainder of the conference.

The 2016 American Institute of Chemical Engineers (AIChE) Annual Meeting. It took place from November 13th to November 18th, 2016 in San Francisco, USA.
In-Silico Tailoring Properties of Polylactide
Alexandr Zubov (Speaker)
Gürkan Sin (Other)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Degree of recognition: International
Links:
https://aiche.confex.com/aiche/2016/webprogram/Paper470226.html

SeaBioGha - Seasonal and spatial variation of seaweed species in Ghana
Period: 7 Nov 2016 – 14 Nov 2016
Marcel Tutor Ale (Other)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Description
Coordinated by Marcel Tutor Ale
Activity: Other

EHEDG World Congress on Hygienic Engineering & Design 2016
Jifeng Yang (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event
EHEDG World Congress on Hygienic Engineering & Design 2016
02/11/2016 – 03/11/2016
Herning, Denmark
Activity: Attending an event › Participating in or organising a conference

Biorefinery Course 28872: Chemical value of a new raw material - Seaweed
Period: 31 Oct 2016
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations
Enzymatisk polymerisation anvendt til fremstilling af biobaserede materialer
Period: 26 Oct 2016
Anders Egede Daugaard (Invited speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Foredrag for Dansk Lak og Farvekemikeres Forening

Documents:
Abstract AED DLFF - short

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Materials Science and Technology 2016
Period: 26 Oct 2016
Adam Paul Karcz (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
Presentation at symposium on Mechanochemical Synthesis and Reaction

Documents:
MST16-APK_v6
Abstract for MST 2016 - v6

Related event
Materials Science and Technology 2016
23/10/2016 → 27/10/2016
Salt Lake City, UT, United States
Activity: Talks and presentations › Conference presentations

Enzymatisk polymerisation anvendt til fremstilling af biobaserede materialer
Anders Egede Daugaard (Invited speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Foredrag for Dansk Lak og Farvekemikeres Forening

Documents:
Abstract AED DLFF - short

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Materials Science and Technology 2016
Adam Paul Karcz (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
Presentation during the Mechanochemical Synthesis and Processing symposium
Degree of recognition: International
Documents:
MST16-APK_v6

Related event

Materials Science and Technology 2016
23/10/2016 → 27/10/2016
Salt Lake City, UT, United States
Activity: Talks and presentations › Conference presentations

Model Based Optimization of an Industrial Wastewater Treatment Plant Combining a Full-scale Granular Sludge Reactor and Autotrophic Nitrogen Removal
Hannah Feldman (Other)
Neda Faraghi Parapari (Other)
Sille Bendix Larsen (Other)
Kasper Kjellberg (Other)
Xavier Flores Alsina (Other)
Gürkan Sin (Other)
Ulf Jeppsson (Other)
Krist V. Gernaey (Other)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Degree of recognition: International

Related event

IWA World Water Congress & Exhibition 2016
09/10/2016 → 14/10/2016
Queensland, Australia
Activity: Talks and presentations › Conference presentations

A Biocatalytic Microreactor – Dynamic CFD Modelling and Experimental Analysis
Period: 27 Sep 2016
Ulrich Krühne (Lecturer)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
Keynote lecture
Documents:
ECCE ECAB3 Nice 2016 Abstract

Related event

3rd European Congress of Applied Biotechnology
27/09/2015 → 01/10/2015
Nice, France
Activity: Talks and presentations › Conference presentations

International Conference on Carbon Dioxide Utilisation 2016
Period: 12 Sep 2016
Rebecca Frauzem (Speaker)
Department of Chemical and Biochemical Engineering

KT Consortium

Description
Oral presentation on one of the days and a participant at the rest of the conference.

The 14th International Conference on Carbon Dioxide Utilization (ICCDU). It took place from September 11th to September 15th, 2016 in Sheffield, UK. It is an annual conference for specialists in carbon dioxide utilization to meet and present new research and ideas.

Related event

International Conference on Carbon Dioxide Utilisation 2016
Sheffield, United Kingdom
Activity: Talks and presentations › Conference presentations

2nd Computational Fluid Dynamics (CFD) and biomass thermochemical Conversion
Period: 9 Sep 2016
Mohammadhadi Nakhaei (Participant)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
The PhD student had a presentation in the workshop and a paper is published as conference proceeding

2nd Computational Fluid Dynamics (CFD) and biomass thermochemical Conversion
Title: CFD simulation of a full-scale RDF-fired calciner
Authors:
Mohammadhadi Nakhaei, Hao Wu, Peter Glarborg, Kim Dam-Johansen
Technical University of Denmark, Department of Chemical and Biochemical Engineering
Lyngby Campus, 2800, Kgs. Lyngby, Denmark
Mnak@kt.dtu.dk, haw@kt.dtu.dk, PGL@kt.dtu.dk, KDJ@kt.dtu.dk

Damien Grévain, Lars Skaarup Jensen
FLSmidth A/S, Cement R&D
Vigerslev Allé 77, 2500 Valby, Denmark
DAG@flsmidth.com, LaSJ@flsmidth.com
ISSN: 2199-9384 ISBN: 978-3-946629-07-8
Documents:
Tagungsband_CFD2016
Links:
(Conference proceeding )

Related event

2nd Computational Fluid Dynamics (CFD) and biomass thermochemical Conversion
09/09/2016 → 09/09/2016
Leipzig, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

20th Nordic Process Control Workshop
Ricardo André Fernandes Caroço (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
Poster contribution
Model-Based Monitoring of an Industrial Batch Pectin Extraction
Documents:
poster_RAFC

Related event

20th Nordic Process Control Workshop
25/08/2016 → 26/08/2016
Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

20th Nordic Process Control Workshop
Riccardo Boiocchi (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

20th Nordic Process Control Workshop
25/08/2016 → 26/08/2016
Sweden
Activity: Talks and presentations › Conference presentations

Sprout Week: summer school
Sofie Kirt Strandbygaard (Other)
KT Consortium
Department of Civil Engineering
Section for Building Design
Description
Summer school in planning around public transport. Reviewer.
Links:
http://sprout.talentweek.dk/

Related external organisation

DAC (Danish Architectural Center)
Strandgade 27B DK, 1401 Copenhagen K, Copenhagen , Denmark
Activity: Other

Catalytic Hydrodeoxygenation of Biomass Pyrolysis Vapor Model Compounds over Molybdenum Sulfide Catalysts: Influence of Support, H2S and Water
Period: Jul 2016
Trine Marie Hartmann Dabros (Guest lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
Description
Poster presentation
Documents:
ICC_TrineArndal_Abstract

Related event

16th International Congress on Catalysis
Thermodynamic modeling of the solubility of silica
Period: 28 Jul 2016
Kaj Thomsen (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Center for Energy Resources Engineering
Centre for oil and gas – DTU
Degree of recognition: International
Documents:
OC25-KajThomsen-Silica

Related event
17th International Symposium on Solubility Phenomena and Related Equilibrium Processes
24/07/2016 → 29/07/2016
Geneva, Switzerland
Activity: Talks and presentations › Conference presentations

Ecotechnologies for wastewater treatment 2016
Riccardo Boiocchi (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event
Ecotechnologies for wastewater treatment 2016
27/07/2016 → 30/07/2016
Activity: Talks and presentations › Conference presentations

Novel high dielectric constant hybrid elastomers based on glycerol-in-silicone emulsions
Period: 3 Jul 2016 → 7 Jul 2016
Piotr Stanislaw Mazurek (Lecturer)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Related event
International Conference on Dielectrics 2016
03/07/2016 → 07/07/2016
Montpellier, France
Activity: Talks and presentations › Conference presentations

Catalytic Hydrodeoxygenation of Biomass Pyrolysis Vapor Model Compounds over Molybdenum Sulfide Catalysts: Influence of Support, H2S and Water
Period: Jun 2016
Trine Marie Hartmann Dabros (Guest lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
**Oral presentation**

Documents:
NordicSymposium_TrineArndal_AbstractOrbit

**Related event**

**17th Nordic Symposium on Catalysis 2016: Surface science and catalysis for sustainable development and the use of large scale facilities for catalysis research**
Period: 14/06/2016 → 16/06/2016
Lund, Sweden

Activity: Talks and presentations › Conference presentations

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**6th International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles**


Aliff Hisyam A Razak (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

**Description**

Electromechanically Active Polymers (EAPs) represent a fast growing and promising scientific field of research and development. EAPs are studied for devices and systems implemented with ‘smart materials’ inherently capable of changing dimensions and/or shape in response to suitable electrical stimuli, so as to transduce electrical energy into mechanical work. They can also operate in reverse mode, transducing mechanical energy into the electrical form. Therefore, they can be used as actuators, mechano-electrical sensors, as well as energy harvesters to generate electricity.

Documents:
EuroEAP 2016_Programme

**Related event**

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**6th International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles: 6th international conference**
Period: 14/06/2016 → 15/06/2016
Helsingør, Denmark

Activity: Attending an event › Participating in or organising a conference

**Glycerol as high-permittivity liquid filler in dielectric silicone elastomers**
Piotr Stanislaw Mazurek (Speaker)

Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

**Description**

Best poster award

Documents:
eaposter_Piotr Mazurek

**Related event**

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**26th European Symposium on Computer-Aided Process Engineering**
Period: 12 Jun 2016 → 15 Jun 2016
Rebecca Frauzem (Participant)

Department of Chemical and Biochemical Engineering
KT Consortium

Description
I participated in the entire duration of the conference.

The annual European Symposium on Computer-Aided Process Engineering. It took place from June 12th to June 15th, 2016 in Portoroz, Slovenia.

Related event

26th European Symposium on Computer-Aided Process Engineering
12/06/2016 → 15/06/2016
Portorož, Slovenia
Activity: Attending an event › Participating in or organising a conference

11th IFAC Symposium on Dynamics and Control of Process Systems Including Biosystems DYCOPS-CAB 2016
Period: 6 Jun 2016 → 8 Jun 2016
Riccardo Boiocchi (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

11th IFAC Symposium on Dynamics and Control of Process Systems Including Biosystems DYCOPS-CAB 2016
06/06/2016 → 08/06/2016
Trondheim, Norway
Activity: Talks and presentations › Conference presentations

24th European Biomass Conference & Exhibition
Guoliang Wang (Participant)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
European Biomass Conference & Exhibition (EUBCE) 2016

Related event

24th European Biomass Conference & Exhibition
06/06/2016 → 09/06/2016
Amsterdam, Netherlands
Activity: Attending an event › Participating in or organising a conference

In-Flame Characterization of a 30 MWth Bio-Dust Flame
Period: 6 Jun 2016
Joakim Myung Johansen (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Related event

24th European Biomass Conference & Exhibition
06/06/2016 → 09/06/2016
Amsterdam, Netherlands
Activity: Talks and presentations › Conference presentations
KT Research Day 2016  
Period: 27 May 2016  
Aliff Hisyam A Razak (Participant)  
Department of Chemical and Biochemical Engineering  
The Danish Polymer Centre  
Description  
Chemical Engineering (KT) Research Day 2016  

Model based monitoring of bioprocessing plants - a solid-liquid extraction example  
Period: 21 Apr 2016  
Ricardo André Fernandes Caroço (Lecturer)  
Department of Chemical and Biochemical Engineering  
CAPEC-PROCESS  

Seaweed Biorefinery in Ghana (SeaBioGha) (External organisation)  
Marcel Tutor Ale (Participant)  
Department of Chemical and Biochemical Engineering  
Center for BioProcess Engineering  
Description  
Work Package Leader  
Degree of recognition: International  
Related external organisation  
Seaweed Biorefinery in Ghana (SeaBioGha)  
Activity: Membership » Membership of research networks or expert groups  

Catalytic liquefaction of lignin to value-added chemicals  
Period: 26 Jan 2016  
Soheila Ghafarnejad Parto (Speaker)  
Jakob Munkholt Christensen (Other)  
Lars Saaby Pedersen (Other)  
Anker Degn Jensen (Other)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre  
Related event  
Workshop on the use of lignocellulosic biomass  
26/01/2016 → …
Odense, Denmark
Activity: Talks and presentations › Conference presentations

12th PSE and 25th ESCAPE Joint Conference
Period: 2015
Seyed Soheil Mansouri (Organizer)
Department of Chemical and Biochemical Engineering

Description
Member of the organizing committee at 12th PSE and 25th ESCAPE joint conference
Links:

Related event
12th PSE and 25th ESCAPE Joint Conference
31/05/2015 → 04/06/2015
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Student Info Meeting
Period: 2015
Marcel Tutor Ale (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related event
Student Info Meeting
01/01/2015 → 01/01/2015
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Annual Polymer Day 2015
Period: 27 Nov 2015
Aliff Hisyam A Razak (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Annual Polymer Day 2015

Related event
Annual Polymer Day 2015: Danish Polymer Centre, Chemical and Biochemical Engineering Department, DTU
27/11/2015 → …
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Role of Industry in a Transition Towards the Bioeconomy in Relation to Biorefinery
Period: 26 Nov 2015
Henning Jørgensen (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Documents:
IEA Task42 Role of industry in transition to BE 2015_HEJR
Links:
http://www.gbs2015.com
Related event

Global Bioeconomy Summit 2015
25/11/2015 → 26/11/2015
Berlin, Germany
Activity: Talks and presentations › Conference presentations

13th Multiphase Flow Conference & Short Course
Period: 24 Nov 2015 → 26 Nov 2015
Jifeng Yang (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

13th Multiphase Flow Conference & Short Course
Dresden, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Biorefining of Seaweed Biomass - Biorefinery DTU Course 28872
Period: 24 Nov 2015
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

A New Optimization Model for Computer-Aided Molecular Design Problems
Period: 9 Nov 2015
Stefano Cignitti (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

2015 AIChE Annual Meeting
08/11/2015 → 13/11/2015
Salt Lake City, United States
Activity: Talks and presentations › Conference presentations

Systematic Computer-Aided Framework for Sustainable Chemical Product Design
Period: 9 Nov 2015
Stefano Cignitti (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Degree of recognition: International

Related event

2015 AIChE Annual Meeting
08/11/2015 → 13/11/2015
Salt Lake City, United States
Activity: Talks and presentations › Conference presentations
2015 AIChE Annual Meeting
Period: 8 Nov 2015 → 13 Nov 2015
Rebecca Frauzem (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
I gave two presentations throughout the course of the conference. In addition, I attended various sessions and events.

I attended and gave two presentations at the AIChE Annual Meeting 2015.

Related event
2015 AIChE Annual Meeting
08/11/2015 → 13/11/2015
Salt Lake City, United States
Activity: Attending an event › Participating in or organising a conference

Biorefining activities in Denmark
Period: 27 Oct 2015
Henning Jørgensen (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related event
IEA Bioenergy Conference 2015: Realising the world's sustainable bioenergy potential
27/10/2015 → 29/10/2015
Berlin, Germany
Activity: Talks and presentations › Conference presentations

Advance Enzyme Technology DTU Course 28247: Extraction of polyphenols from apple using cell wall degrading enzymes
Period: 19 Oct 2015
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Combustion Characterization of Individual Bio-oil Droplets
Period: 7 Oct 2015
Brian Brun Hansen (Lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Related event
The Nordic Flame Days 2015
06/10/2015 → 07/10/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations
The Nordic Flame Days 2015
Period: 6 Oct 2015
Sunday Chukwudi Okoro (Speaker)
Materials and Surface Engineering
Department of Mechanical Engineering
CHEC Research Centre

Description
Alkali chloride induced corrosion of superheaters under biomass firing conditions: Improved insights from laboratory scale studies

Related event
The Nordic Flame Days 2015
06/10/2015 → 07/10/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

The Nordic Flame Days 2015
Guoliang Wang (Participant)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
Nordic Flame Days 2015
Links:
http://flamedays2015.sfrc.se/

Related event
The Nordic Flame Days 2015
06/10/2015 → 07/10/2015
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

10th European Congress of Chemical Engineering
Period: 28 Sep 2015 → 29 Sep 2015
Rebecca Frauzem (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
I presented a poster at the conference.

Participation in the European Congress on Chemical Engineering 2015.

Related event
10th European Congress of Chemical Engineering
27/09/2015 → 01/10/2015
Nice, France
Activity: Attending an event › Participating in or organising a conference

A Systematic Computer-Aided Framework for Integrated Design and Control of Chemical Processes
Period: 28 Sep 2015
Seyed Soheil Mansouri (Keynote speaker)
Department of Chemical and Biochemical Engineering

CAPEC-PROCESS

Description
Chemical processes are conventionally designed through a sequential approach. In this sequential approach, first, a steady-state process design is obtained and then, control structure synthesis that, in most of the cases, is based on heuristics is performed. Therefore, process design and process control and operation considerations have been studied independently. Furthermore, this sequential approach does not adequately answer this question, "How process design decisions influence process control and operation?". In order to answer this question, it is necessary to consider process controllability and operability issues together with process design tasks (Seferlis and Georgiadis, 2004). In this way, it can be assured that design decisions give the optimum operational and economic performance. Operability issues are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions.

In this work, a systematic hierarchical computer-aided framework for integrated process design and control of chemical processes including process intensification is proposed. Note however, because of integration of functions/operations into one system the controllability region of intensified equipment may become smaller (Nikačević et al., 2012). The methodology developed in this work, employs a decomposition-based approach so that the complexity of the problem is reduced into a set of sub-problems that are solved sequentially. The production of methy-tert-butyl-ether (MTBE) is used to demonstrate the application of the framework. First, optimal design-control solution is presented for MTBE production via a reactor-separator-recycle (RSR) system. Next, it will be shown that the RSR system can be replaced by an intensified unit operation, a reactive distillation column (RDC) which optimal design-control solution is also presented. The operation and control of the RSR and RDC at the optimal designs is compared with other candidate designs compared through open-loop and closed-loop analysis. By application of this methodology it is shown that the optimal design obtained from this methodology, it is not only the best from an economic steady-state design point of view, but also from control and operation point view. It is verified that the optimal design options for RSR and RDC are less sensitive to the disturbances in the feed at the optimal design.

Related event

10th European Congress of Chemical Engineering
27/09/2015 → 01/10/2015
Nice, France
Activity: Talks and presentations › Conference presentations

Period: 28 Sep 2015
Stefano Cignitti (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

10th European Congress of Chemical Engineering
27/09/2015 → 01/10/2015
Nice, France
Activity: Talks and presentations › Conference presentations

10th European Congress of Chemical Engineering
Period: 27 Sep 2015 → 1 Oct 2015
Zainatul Bahiyah Handani (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
Optimal synthesis and design of integrated process and wastewater treatment networks

Related event

10th European Congress of Chemical Engineering
27/09/2015 → 01/10/2015
Nice, France
Activity: Attending an event › Participating in or organising a conference

**Training School on Dielectric Elastomer Transducers 2015**
*Period: 8 Sep 2015 → 10 Sep 2015*
Piotr Stanislaw Mazurek (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

**Description**
Training School on Dielectric Elastomer Transducers 2015

**Related event**

**Training School on Dielectric Elastomer Transducers 2015**
08/09/2015 → 10/09/2015
Neuchatel, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**ESNAM training school 2015**
*Period: 7 Sep 2015 → 11 Sep 2015*
Aliff Hisyam A Razak (Participant)
Department of Chemical and Biochemical Engineering

**Description**
Training school Dielectric elastomer transducers
Documents:
TS2015 neuchatel v5 xlsx_schedule

**Related event**

**ESNAM training school 2015**
07/09/2015 → 11/09/2015
Neuchatel, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**4th Summer School of the IMPRS Magdeburg on Process Systems Engineering**
*Period: 31 Aug 2015 → 4 Sep 2015*
Stefano Cignitti (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

**Related event**

**4th Summer School of the IMPRS Magdeburg on Process Systems Engineering**
31/08/2015 → 04/09/2015
Magdeburg, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Dynamic Modeling and Optimization of Large Scale Lignocellulosic Biorefineries**
*Period: 18 Aug 2015*
Remus Mihail Prunescu (Invited speaker)
Department of Electrical Engineering
Automation and Control
Department of Chemical and Biochemical Engineering
Related event

BioPro World Talent Campus 2015
17/08/2015 → 21/08/2015
Sore, Denmark
Activity: Talks and presentations › Conference presentations

Gordon Research Seminar on Cellulosomes, Cellulases & Other Carbohydrate Modifying Enzymes
Period: 1 Aug 2015 → 2 Aug 2015
Casper Wilkens (Invited speaker)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related event

Gordon Research Seminar on Cellulosomes, Cellulases & Other Carbohydrate Modifying Enzymes : A New Era of Research on Carbohydrate-Active Enzymes: Their Reaction Mechanisms and Evolution
01/11/2015 → 02/11/2015
Andover, United States
Activity: Talks and presentations › Conference presentations

Gordon Research Conference on High Temperature Corrosion
Sunday Chukwudi Okoro (Participant)
Materials and Surface Engineering
Department of Mechanical Engineering
CHEC Research Centre
Department of Chemical and Biochemical Engineering

Related event

Gordon Research Conference on High Temperature Corrosion
26/07/2015 → 31/07/2015
New London, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

9th IWA Symposium on Systems Analysis and Integrated Assessment (Watermatex 2015)
Riccardo Boiocchi (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

9th IWA Symposium on Systems Analysis and Integrated Assessment (Watermatex 2015)
14/06/2015 → 17/06/2015
Gold Coast, Queensland, Australia
Activity: Talks and presentations › Conference presentations

29th International Conference on Surface Modification Technologies
Period: 11 Jun 2015
Sunday Chukwudi Okoro (Speaker)
Materials and Surface Engineering
Department of Mechanical Engineering
CHEC Research Centre
Department of Chemical and Biochemical Engineering

Description
Improving the high-temperature corrosion resistance of alumina forming alloys under biomass-firing conditions by pre-oxidizing the surface

Related event
29th International Conference on Surface Modification Technologies
10/06/2015 → 12/06/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles
Period: 9 Jun 2015 → 10 Jun 2015
Piotr Stanislaw Mazurek (Participant)

Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Presenting a poster of "Enhancing relative permittivity by incorporating PDMS-PEG multiblock copolymer in the binary polymer blends"

Related event
5th International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles
09/06/2015 → 10/06/2015
Tallinn, Estonia
Activity: Attending an event › Participating in or organising a conference

Experimental analysis of a solid oxide fuel cell stack coupled with biomass gasification
Period: 3 Jun 2015
Rasmus Østergaard Gadsbøll (Speaker)

Department of Chemical and Biochemical Engineering
CHEC Research Centre

Related event
European Biomass Conference & Exhibition 2015
01/06/2015 → …
Vienna, Austria
Activity: Talks and presentations › Conference presentations
Nordic Polymer Days 2015
Period: 1 Jun 2015 → 3 Jun 2015
Piotr Stanislaw Mazurek (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Preparing mono-dispersed liquid core PDMS microcapsules from thiol–ene–epoxy-tailored flow-focusing microfluidic devices
Documents:
Abstract NPD_Piotr Mazurek

Related event
Nordic Polymer Days 2015
08/06/2015 → 10/06/2015
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Nordic Polymer Days 2015
Period: 1 Jun 2015 → 3 Jun 2015
Aliff Hisyam A Razak (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Presenting 15 min speech about "Enhancing relative permittivity by incorporating PDMS-PEG multiblock copolymer in binary polymer blends"

IDA Polymer is the organizer of the 52nd Nordic Polymer Days in 2015. This traditional annual event is a golden opportunity for researchers especially PhD students to present their work either as a short oral presentation or as a poster.

Related event
Nordic Polymer Days 2015
08/06/2015 → 10/06/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

12th PSE and 25th ESCAPE Joint Conference
Stefano Cignitti (Organizer)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
Co-organizer
Links:

Related event
12th PSE and 25th ESCAPE Joint Conference
31/05/2015 → 04/06/2015
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference
12th PSE and 25th ESCAPE Joint Conference
Riccardo Boiocchi (Participant)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event
12th PSE and 25th ESCAPE Joint Conference
31/05/2015 → 04/06/2015
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

25th European Symposium on Computer Aided Process Engineering
Rebecca Frauzem (Organizer)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
As part of the organizing team, I was in charge of ensuring that everything ran smoothly during the conference. In addition, I was a member of the editors for the book of abstracts. Finally, I helped in planning everything beforehand with a group of colleagues.

Organization of PSE2015/ESCAPE25 conference in Copenhagen.

Related event
31/05/2015 → 04/06/2015
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Multivariate analysis of industrial scale fermentation data
Lisa Mears (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event
12th PSE and 25th ESCAPE Joint Conference
31/05/2015 → 04/06/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

4th International Congress on Sustainability Science & Engineering
Period: 28 May 2015
Rebecca Frauzem (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
Gave an oral presentation at the ICOSSE 2015 Conference.

Related event
4th International Congress on Sustainability Science & Engineering  
26/05/2015 → 29/05/2015  
Balatonfüred, Hungary  
Activity: Talks and presentations › Conference presentations

Zainatul Bahiyah Handani (Participant)  
Department of Chemical and Biochemical Engineering  
CAPEC-PROCESS

Description  
Early Stage Synthesis and Design of Integrated Process and Wastewater Treatment Networks

Related event

4th International Congress on Sustainability Science & Engineering  
26/05/2015 → 29/05/2015  
Balatonfüred, Hungary  
Activity: Attending an event › Participating in or organising a conference

Application of Multivariate Analysis Tools to Industrial Scale Fermentation Data  
Period: 22 Apr 2015 → 24 Apr 2015  
Lisa Mears (Speaker)  
Department of Chemical and Biochemical Engineering  
CAPEC-PROCESS

Related event

Advances in Process Analytics and Control Technology  
22/04/2015 → 24/04/2015  
Manchester, United Kingdom  
Activity: Talks and presentations › Conference presentations

Linear viscoelastic characterization from filament stretching rheometry  
Period: 16 Apr 2015  
Sara Lindeblad Wingstrand (Speaker)  
Department of Chemical and Biochemical Engineering  
The Danish Polymer Centre  
Links:  

Related event

10th Annual European Rheology Conference: Golden Jubilee Meeting of Groupe Français de Rhéologie  
14/04/2015 → 17/09/2015  
Nantes, France  
Activity: Talks and presentations › Conference presentations

Climate-CAFE programme meeting  
Period: 4 Feb 2015 → 6 Feb 2015  
Teis Nørgaard Mikkelsen (Participant)  
Ecosystems Programme  
Department of Chemical and Biochemical Engineering

Description  
Facilities for Ecosystem manipulating: Methods under the Climate-CAFE programme - Toulouse France
The DTU Risø based facilities for ecosystem manipulating was presented for the international participant group

Related event

**Climate-CAFE programme meeting**
04/02/2015 → 06/02/2015
Toulouse, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**19th Nordic Process Control Workshop**
Period: 13 Jan 2015 → 16 Jan 2015
Riccardo Boiocchi (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

**19th Nordic Process Control Workshop**
13/01/2015 → 16/01/2015
Trondheim, Norway
Activity: Talks and presentations › Conference presentations

**Presentation for Seaweed Biorefinery in Ghana (SeaBioGha) - Danida funded project (External organisation)**
Period: 11 Jan 2015 → 26 Jan 2015
Marcel Tutor Ale (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related external organisation

**Presentation for Seaweed Biorefinery in Ghana (SeaBioGha) - Danida funded project**
Activity: Membership › Membership of research networks or expert groups

**Student Info Meeting**
Period: 2014
Marcel Tutor Ale (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related event

**Student Info Meeting**
01/01/2014 → 01/01/2014
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Annual Polymer Day 2014: Oral presentation**
Period: 21 Nov 2014
Aliff Hisyam A Razak (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Research, knowledge-sharing and development was in focus when DPC hosted the 10th Annual Polymer Day on 21 November.
Documents:
Annual Polymer Day 2014 - Agenda
Related event

10th Annual Polymer Day
21/11/2014 → 21/11/2014
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

2014 AIChE Annual Meeting: American Institute of Chemical Engineers
Period: 19 Nov 2014
Rebecca Frauzem (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
Gave an oral presentation at the AIChE Annual Meeting 2014.

Related event

2014 AIChE Annual Meeting: American Institute of Chemical Engineers
16/11/2014 → 21/11/2014
Atlanta, United States
Activity: Talks and presentations › Conference presentations

Dynamic Simulation, Sensitivity and Uncertainty Analysis of a Demonstration Scale Lignocellulosic Enzymatic Hydrolysis Process
Period: 16 Nov 2014 → 21 Nov 2014
Remus Mihail Prunescu (Speaker)
Department of Electrical Engineering
Automation and Control
CAPEC-PROCESS
Department of Chemical and Biochemical Engineering

Related event

2014 AIChE Annual Meeting: American Institute of Chemical Engineers
16/11/2014 → 21/11/2014
Atlanta, United States
Activity: Talks and presentations › Conference presentations

Biorefinery DTU Course 28872: Seaweed Biorefinery
Period: 31 Oct 2014
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Climate change and ozone toxicity in plants
Teis Nørgaard Mikkelsen (Lecturer)
Department of Chemical and Biochemical Engineering
Ecosystems Programme
4th ECLAIRE General Assembly and Annual Meeting
Period: 28 Sep 2014 → 30 Sep 2014
Teis Nørgaard Mikkelsen (Participant)
Department of Chemical and Biochemical Engineering
Ecosystems Programme

Microfluidics in Chemical and Biochemical Engineering Applications
Period: 23 Sep 2014
Ulrich Krühne (Lecturer)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

European Corrosion Congress
Period: 8 Sep 2014 → 12 Sep 2014
Sunday Chukwudi Okoro (Speaker)
Materials and Surface Engineering
Department of Mechanical Engineering
CHEC Research Centre
Department of Chemical and Biochemical Engineering

An integrated approach for synthesis and design of process and water/wastewater networks
Zainatul Bahiyah Handani (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
Abstract from 21st International Congress of Chemical and Process Engineering CHISA 2014 Prague

Related event
21st International Congress of Chemical and Process Engineering
23/08/2014 → 27/08/2014
Prague, Czech Republic
Activity: Talks and presentations › Conference presentations

The role of oxidative enzymes during enzymatic hydrolysis of lignocellulosic material at industrial conditions
Period: 22 Jul 2014
Henning Jørgensen (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related event
Society for Industrial Microbiology and Biotechnology Annual Meeting 2014
20/07/2014 → 24/07/2014
St. Louis, United States
Activity: Talks and presentations › Conference presentations

A Comparative Study of Two Full-Scale Swirl Stabilized Bio-Dust Power Plant Flames
Period: 24 Jun 2014
Joakim Myung Johansen (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
Documents:
biomass energy conference - abstract
supplementary material

Related event
22nd European Biomass Conference and Exhibition
23/06/2014 → 26/06/2014
Hamburg, Germany
Activity: Talks and presentations › Conference presentations

International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles
Period: 10 Jun 2014 → 11 Jun 2014
Shamsul Bin Zakaria (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Poster presentation
Links:

Related event
4th International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles
10/06/2014 → 11/06/2014
Linköping, Sweden
Activity: Attending an event › Participating in or organising a conference

**International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles**
**Period:** 10 Jun 2014 → 11 Jun 2014
**Aliff Hisyam A Razak (Participant)**

The Danish Polymer Centre
Department of Chemical and Biochemical Engineering

Links:

**Related event**

**4th International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles**
**10/06/2014 → 11/06/2014**
**Linköping, Sweden**

Activity: Attending an event › Participating in or organising a conference

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**A free air in situ ozone fumigation system designed for partial plant exposure**
**Period:** 18 May 2014 → 22 May 2014
**Teis Nørgaard Mikkelsen (Lecturer)**

Department of Chemical and Biochemical Engineering
Ecosystems Programme

**Description**
Foredrag afholdt ved "International conference on ozone and plants".

**Related event**

**International conference on ozone and plants**
**18/05/2014 → 21/05/2014**
**Beijing, China**

Activity: Talks and presentations › Conference presentations

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**Long term acclimation to elevated CO2 and drought increases the ozone toxicity in plants**
**Period:** 18 May 2014 → 22 May 2014
**Teis Nørgaard Mikkelsen (Lecturer)**

Department of Chemical and Biochemical Engineering
Ecosystems Programme

**Description**
Participation in "International conference on ozone and plants".

**Related event**

**International conference on ozone and plants**
**18/05/2014 → 21/05/2014**
**Beijing, China**

Activity: Talks and presentations › Conference presentations

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**Karakterisering af partikler fra brændeovne, herunder black carbon**
**Period:** 29 Apr 2014
**Brian Brun Hansen (Lecturer)**

Department of Chemical and Biochemical Engineering
CHEC Research Centre

**Related event**
Pretreatment for cellulosic ethanol production in the developing world

Period: 28 Apr 2014 → 1 May 2014
Sune Tjalfe Thomsen (Lecturer)

Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Description
In the context of the Developing World, it is challenging to implement technological schemes with large-scale, high-performance technologies, due to i.e. the poor biomass infrastructure, which in most cases are not able to support collection, storage and transport of huge amounts of the biomass needed for a large-scale facility. Therefore, pretreatment for cellulosic ethanol should be optimized within the constraints of a smaller scale than envisioned in most scientific studies. On the other hand, it might be conceivable to employ methods that are more labor intensive than methods developed for the industrialized world. In the current study, a thorough investigation of three alternative pretreatment methods applicable for small-scale low-tech conditions is described (boiling pretreatment, soaking in aqueous ammonia, and white rot fungi pretreatment). These methods are benchmarked against well-known hydrothermal treatment. The pretreatments is tested on 11 West African biomasses, i.e. cassava stalks, plantain peelings, plantain trunks, plantain leaves, cocoa husks, cocoa pods, maize cobs, maize stalks, rice straw, groundnut straw and oil palm empty fruit bunches. The raw and pretreated biomasses are screened in an enzymatic convertibility assay where after the most promising biomasses are subjected to compositional analysis and ethanol fermentation. We find that the alternative methods are viable, especially when looking at the overall utilization of the biomasses, even though only less than half of the tested biomasses are suitable for cellulosic ethanol production with sufficiently high yields. Furthermore, we elaborate on the mode of action of the pretreatment methods and their effect on the different biomasses.

Related event
36th Symposium on Biotechnology for Fuels and Chemicals
28/04/2014 → 01/05/2014
Clearwater Beach, FL, United States
Activity: Talks and presentations › Conference presentations

Microscopy of Oxidation
Period: 14 Apr 2014 → 16 Apr 2014
Sunday Chukwudi Okoro (Participant)

Department of Chemical and Biochemical Engineering
CHEC Research Centre
Department of Mechanical Engineering
Materials and Surface Engineering

Description
Poster Presentation

Related event
Microscopy of Oxidation
14/04/2014 → 16/04/2014
Nottingham, United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

46th American Air pollution workshop
Period: 7 Apr 2014 → 10 Apr 2014
Teis Nørgaard Mikkelsen (Speaker)
Department of Chemical and Biochemical Engineering
Ecosystems Programme

Description
Long term acclimation to elevated CO2 and drought increases the ozone toxicity in plants.

46th American Air pollution workshop, Guadalajara, Mexico.

Related event

46th American Air pollution workshop
07/04/2014 → 10/04/2014
Guadalajara, Mexico
Activity: Talks and presentations › Conference presentations

Local Measurements in Two Full-Scale Swirl Stabilized Bio-Dust Burners: A Parametric Study
Period: 27 Mar 2014
Joakim Myung Johansen (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
Documents:
Combustion_Template_latex

Related event

Joint meeting of the British and Scandinavian-Nordic Sections of the Combustion Institute
27/03/2014 → 28/03/2014
Cambridge, United Kingdom
Activity: Talks and presentations › Conference presentations

ESNAM Training School 2014
Period: 25 Mar 2014 → 27 Mar 2014
Aliff Hisyam A Razak (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Dielectric elastomers training school

Related event

ESNAM Training School 2014
25/03/2014 → 27/03/2014
Darmstadt, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

BreedFACE
Period: 19 Mar 2014
Teis Nørgaard Mikkelsen (Invited speaker)
Department of Chemical and Biochemical Engineering
Ecosystems Programme

Description
Past, present, future FACE activities in Jülich, Germany.

FACE systems for breeding and diversity of genetic and molecular responses to elevated CO2.

Related event
BreedFACE  
19/03/2013 → 20/03/2014  
Jülich, Germany  
Activity: Talks and presentations › Conference presentations

SPIE Smart Structures/NDE  
Period: 9 Mar 2014 → 13 Jun 2014  
Shamsul Bin Zakaria (Participant)  
Department of Chemical and Biochemical Engineering  
The Danish Polymer Centre  
Description  
poster presentation

Related event  
SPIE Smart Structures/NDE: Smart Structures and Materials & Nondestructive Evaluation and Health Monitoring  
09/03/2014 → 13/03/2014  
San Diego, CA, United States  
Activity: Attending an event › Participating in or organising a conference

Recent progress on biofuel commercialization activities in Denmark  
Period: 21 Jan 2014  
Henning Jørgensen (Lecturer)  
Department of Chemical and Biochemical Engineering  
Center for BioProcess Engineering  
Related event  
11th International Conference on Biofuels: Fuels of the future 2014  
20/01/2014 → 21/01/2014  
Berlin, Germany  
Activity: Talks and presentations › Conference presentations

Kitasato University Hospital  
Period: 2013  
Marcel Tutor Ale (Visiting researcher)  
Department of Chemical and Biochemical Engineering  
Center for BioProcess Engineering  
Description  
Bioactivity of polysaccharides from seaweed and tragacant  
Anti-cancer activity assay and immune response of fucoidan and tragacant by natural killer cells activity assay.  
Activity: Visiting an external institution › Visiting another research institution

Student Info Meeting  
Period: 2013  
Marcel Tutor Ale (Participant)  
Department of Chemical and Biochemical Engineering  
Center for BioProcess Engineering  
Related event  
Student Info Meeting  
01/01/2013 → 01/01/2013  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
2nd Symposium on Applied Synthetic Biology in Europe  
**Period:** 25 Nov 2013 → 27 Nov 2013  
Yao Guo (Participant)  
Department of Chemical and Biochemical Engineering  
Center for BioProcess Engineering  

**Description**  
Oral presentation: Enzymatic production of human milk oligosaccharides.  
Documents:
C:\Users\yagu\Documents\Backup personal drive\project\Meetings and Seminars\20131125-27 Malaga\conference in Malaga\Abstract_Form_distributed_CONFERENCE MALAGA

**Related event**

2nd Symposium on Applied Synthetic Biology in Europe  
Period: 25/11/2013 → 27/11/2013  
Malaga, Spain  
Activity: Attending an event › Participating in or organising a conference

**9th Annual Polymer Day**  
**Period:** 22 Nov 2013  
Aliff Hisyam A Razak (Participant)  
Department of Chemical and Biochemical Engineering  
The Danish Polymer Centre  

**Description**  
Annual Polymer Day 2013  

**Related event**

9th Annual Polymer Day  
Period: 22/11/2013 → 22/11/2013  
Kgs. lyngby, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**The Electrical Breakdown of Thin Dielectric Elastomers: Thermal Effects**  
**Period:** 22 Nov 2013  
Shamsul Bin Zakaria (Speaker)  
Department of Chemical and Biochemical Engineering  
The Danish Polymer Centre  

**Related event**

9th Annual Polymer Day  
Period: 22/11/2013 → 22/11/2013  
Kgs. lyngby, Denmark  
Activity: Talks and presentations › Conference presentations

**KALIBRERING af IR TERMOMETRE: Betydning af afstand, apertur, opvarmning, IR termometer kvalitet, etc.**  
**Period:** 20 Nov 2013  
Sønnik Clausen (Invited speaker)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre  

**Description**  
Teknisk Kommite for Akkrediteret Kalibrering.
Advance Enzyme Technology DTU Course 28247: Effect of enzyme on the release of phenolics and rheology of apple mash.
Period: 18 Nov 2013
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Biorefinery DTU Course 28872: Seaweed as a raw material
Period: 8 Nov 2013
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

ESNAM Training School on Ionic Artificial Muscles
Piotr Stanislaw Mazurek (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

BINARY VLE of DEEA/H2O, MAPA/H2O and DEEA/MAPA SYSTEMS
Period: 5 Jun 2013
Muhammad Waseem Arshad (Speaker)
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering

Description
Oral Presentation by Ardi Hartono, Fahad Saleem, Muhammad Waseem Arshad, Muhammad Usmana and Hallvard F. Svendsen
Documents:
prod21371141562601.Ardi_Waseem_TCCS7_Final.pdf
**Related event**

**7th Trondheim CCS Conference**
04/06/2013 → 06/06/2013
Trondheim, Norway
Activity: Talks and presentations › Conference presentations

**Datalogning: Hvordan aflæser du din Temperatur**
Period: 4 Jun 2013
Mogens Kirkegaard (Lecturer)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

**Description**
Temperatur teori, kalibrering af loggere, temperatur mapping.

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**In-Flame Measurements on Full-Scale Swirl Stabilized Bio-Dust Burners at Different Operational Conditions**
Period: 3 Jun 2013 → 7 Jun 2013
Joakim Myung Johansen (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

**Documents:**
biomass energy conference - abstract
supplementary material

**Related event**

**EU BC&E 21st European Biomass Conference and Exhibition**
03/06/2013 → 07/06/2013
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**8th Danish Conference on Biotechnology and Molecular Biology**
Period: 30 May 2013 → 31 May 2013
Yao Guo (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

**Description**
Poster presentation.

**Related event**

**8th Danish Conference on Biotechnology and Molecular Biology: Food Biotechnology and Nutigenomics**
30/05/2013 → 31/05/2013
Vejle, Denmark
Activity: Attending an event › Participating in or organising a conference

**Increase**
Period: 24 May 2013
Teis Nørgaard Mikkelsen (Speaker)
Department of Chemical and Biochemical Engineering
Ecosystems Programme

**Description**
Improving the performance of infrared reflective night curtains for warming field plots.

**INCREASE Project meeting in Copenhagen.**

**Related event**
Increase : Improving the performance of infrared reflective night curtains for warming field plots
23/05/2013 → 24/05/2013
København, Denmark
Activity: Other

**4th Laboratory Course on Dielectric Spectroscopy**
Period: 20 May 2013 → 24 May 2013
Piotr Stanislaw Mazurek (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

**Related event**
4th Laboratory Course on Dielectric Spectroscopy
20/05/2013 → 24/05/2013
San Sebastian, Spain
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**A Tool to Support Optimal Industrial Wastewater Treatment Design and Analysis**
Period: 24 Apr 2013 → 26 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

**Description**

**Related event**
Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Activity: Talks and presentations › Conference presentations

**A Tool to Support Optimal Industrial Wastewater Treatment Design and Analysis**
Period: 24 Apr 2013 → 26 Apr 2013
Hande Bozkurt (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

**Description**

**Related event**
Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Activity: Talks and presentations › Conference presentations

A Tool to Support Optimal Industrial Wastewater Treatment Design and Analysis
Period: 24 Apr 2013 → 26 Apr 2013
Gürkan Sin (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering

Description

Related event
Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Activity: Talks and presentations › Conference presentations

Design of future municipal wastewater treatment plants: A mathematical approach to manage complexity and identify optimal solutions
Period: 24 Apr 2013 → 26 Apr 2013
Hande Bozkurt (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description

Related event
Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Activity: Talks and presentations › Conference presentations
Design of future municipal wastewater treatment plants: A mathematical approach to manage complexity and identify optimal solutions
Period: 24 Apr 2013 → 26 Apr 2013
Krist V. Gernaey (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering
Center for Process Engineering and Technology

Description

Related event

Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Activity: Talks and presentations › Conference presentations

Design of future municipal wastewater treatment plants: A mathematical approach to manage complexity and identify optimal solutions
Period: 24 Apr 2013 → 26 Apr 2013
Gürkan Sin (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering

Description

Related event

Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Activity: Talks and presentations › Conference presentations

Selection and design of solvents
Period: 21 Apr 2013 → 24 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Oral conference presentation: Rafiqul Gani, 2013, “Selection and design of solvents”, Plenary Lecture

Related event

23rd Croatian Meeting of Chemists and Chemical Engineers
21/04/2013 → 24/04/2013
Osijek, Croatia
Activity: Talks and presentations › Conference presentations

Computer-aided modeling framework: a generic template as a modeling tool
Period: 20 Apr 2013 → 25 Apr 2013
Marina Fedorova (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Computer-aided modeling framework: a generic template as a modeling tool
Period: 20 Apr 2013 → 25 Apr 2013
Gürkan Sin (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering

Description

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology
Period: 20 Apr 2013 → 25 Apr 2013
Georgios Kontogeorgis (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Center for Energy Resources Engineering
Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology
Period: 20 Apr 2013 → 25 Apr 2013
Michele Mattei (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Center for Energy Resources Engineering
CERE – Center for Energy Resources Engineering

Description
Oral conference presentation: Michele Mattei, Peter Krogh, Bo Depner, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, “Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology”

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Efficient Information and Data Management in Synthesis and Design of Processing Networks
Period: 20 Apr 2013 → 25 Apr 2013
Gürkan Sin (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering

Description
Oral Conference Presentation: A. Quaglia, G. Sin, R. Gani, 2013, "Efficient Information and Data Management in Synthesis and Design of Processing Networks"

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Efficient Information and Data Management in Synthesis and Design of Processing Networks
Period: 20 Apr 2013 → 25 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering

Description
Oral Conference Presentation: A. Quaglia, G. Sin, R. Gani, 2013, "Efficient Information and Data Management in Synthesis and Design of Processing Networks"

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel
Period: 20 Apr 2013 → 25 Apr 2013
Larissa Cunico (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Oral Conference Presentation: Larissa P. Cunico, Roberta Ceriani, Bent Sarup, Rafiqul Gani, 2013, "Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel"

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel
Period: 20 Apr 2013 → 25 Apr 2013
Roberta Ceriani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Oral Conference Presentation: Larissa P. Cunico, Roberta Ceriani, Bent Sarup, Rafiqul Gani, 2013, "Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel"
Related event

9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel
Period: 20 Apr 2013 → 25 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Oral Conference Presentation: Larissa P. Cunico, Roberta Ceriani, Bent Sarup, Rafiqul Gani, 2013, “Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel”

Related event

9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Kitasato University Hospital
Period: 2012
Marcel Tutor Ale (Visiting researcher)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Description
Evaluation of fucoidan anti-cancer activity on melanoma and lung cancer cells

Anti-cancer activity assay and immune response of fucoidan by natural killer cells activity assay.
Activity: Visiting an external institution › Visiting another research institution

Student Info Meeting
Period: 2012
Marcel Tutor Ale (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Description
Student Info Meeting

Related event

Student Info Meeting
01/01/2012 → 01/01/2012
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Recent advances in CAPE and PSE applicable to the Pharmaceuticals Industry
Period: 19 Dec 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

8th Annual Polymer Day
Period: 30 Nov 2012
Sindhu Vudayagiri (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Description
'Hot-embossing of Microstructures on addition-curing PDMS films'

Related event

Computational Solvent Design for Integrated Chemical Processes
Period: 15 Nov 2012 → 16 Nov 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Advance Enzyme Technology DTU Course 28247: Extraction of polyphenols from apple using enzymes
Period: 14 Nov 2012
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Pesticide uptake modeling
Period: 7 Nov 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description
Rafiquul Gani, 2012, “Pesticide uptake modeling”, Syngenta, Jealott’s International Research Centre, UK, 7 November

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

The Continuous Chromatographic Separation of Molecules/Particles Using Optical Electric Fields
Period: 30 Oct 2012
Nicolas Javier Alvarez (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Documents:
Optical_Field_Chromatography.pdf

Related event

2012 AIChE Annual Meeting: Cleaner Energy, Stronger Economy, Better Living
28/10/2012 → 02/11/2012
Pittsburgh, PA, United States
Activity: Talks and presentations › Conference presentations

Constant Elongational Stress Measurements of LDPE and PS Using a Filament Stretching Rheometer
Period: 29 Oct 2012
Nicolas Javier Alvarez (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Related event

2012 AIChE Annual Meeting: Cleaner Energy, Stronger Economy, Better Living
28/10/2012 → 02/11/2012
Pittsburgh, PA, United States
Activity: Talks and presentations › Conference presentations

Separation of Macromolecules by Photonic Crystal Defects Chromatography (PCDC)
Period: 28 Oct 2012
Nicolas Javier Alvarez (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Related event

2012 AIChE Annual Meeting: Cleaner Energy, Stronger Economy, Better Living
28/10/2012 → 02/11/2012
Pittsburgh, PA, United States
Activity: Talks and presentations › Conference presentations

Biorefinery DTU Course 28872 - Chemical Value of new raw material: ALGAE
Period: 30 Sep 2012
Marcel Tutor Ale (Lecturer)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related external organisation

Unknown external organisation
Research at CAPEC
Period: 27 Sep 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Rafiqul Gani, 2012, “Research at CAPEC”, Mitsubishi Research Center, Mizushima, Japan, 27 September

Related external organisation

Material design and processing – hard competition or great synergy?
Period: 19 Sep 2012
Anne Ladegaard Skov (Lecturer)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Related event
Materiality of Light: Designing With Light And Energy Flows
19/09/2012 → 21/09/2012
Copenhagen, Denmark

Silicon days
Period: 5 Sep 2012
Sindhu Vudayagiri (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Hot-Embossing of microstructures on addition-curing PDMS films, Oral presentation

Related event
Silicon days
05/09/2012 → …
Lyon, France

International Conference on Operations Research
Period: 2 Sep 2012
Klaus Reinholdt Nyhuus Hansen (Participant)
Production and Service Management
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Links:
http://www.or2011.ch/index (Conference website.)
**Related event**

**International Conference on Operations Research**  
30/08/2011 → 02/09/2011  
Zürich, Switzerland  
Activity: Attending an event › Participating in or organising a conference

The continuous separation of molecules on the basis of their polarizability using optical electric fields  
Period: 7 Aug 2012  
Nicolas Javier Alvarez (Speaker)  
Department of Chemical and Biochemical Engineering  
The Danish Polymer Centre

**16th International Conference on Rheology**  
05/08/2012 → 10/08/2012  
Lisbon, Portugal  
Activity: Talks and presentations › Conference presentations

Release of K, Cl, and S during Combustion and Co-Combustion with Wood of High-Chlorine biomass in Bench and Pilot Scale  
Period: 31 Jul 2012  
Joakim Myung Johansen (Speaker)  
Department of Chemical and Biochemical Engineering  
CHEC Research Centre

**34th International Symposium on Combustion**  
29/07/2012 → 03/08/2012  
Warsaw, Poland  
Activity: Talks and presentations › Conference presentations

Amol Shivajirao Hukkerikar (Speaker)  
Department of Chemical and Biochemical Engineering  
Computer Aided Process Engineering Center

**Description**  

**Related event**

**11th International Symposium on Process Systems Engineering**  
15/07/2012 → 19/07/2012  
Singapore  
Activity: Talks and presentations › Conference presentations

**25th European Conference on Operations Research**  
Period: 10 Jul 2012  
Klaus Reinholdt Nyhuus Hansen (Participant)  
Production and Service Management
Description
Links:
http://www.euro-2012.lt/welcome (Conference webpage.)

Related event
25th European Conference on Operations Research: OR Connecting Sciences
08/07/2012 → 11/07/2012
Vilnius, Lithuania
Activity: Attending an event › Participating in or organising a conference

8th Coatings Science International
Period: 28 Jun 2012
Kristian Petersen Nørgaard (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre
Description
Poster presentation
Poster at 8th Coating Science International, Noordwijk, The Netherlands
Related event
8th Coatings Science International
25/06/2012 → 29/06/2012
Noordwijk, Netherlands
Activity: Talks and presentations › Conference presentations

The continuous separation of molecules on the basis of their polarizability using optical electric fields
Period: 19 Jun 2012
Nicolas Javier Alvarez (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Documents:
Text file
Related event
6th Conference of the International Marangoni Association: Interfacial Fluid Dynamics and Processes
18/06/2012 → 22/06/2012
Haifa, Israel
Activity: Talks and presentations › Conference presentations

Thermocapillary instability of three immiscible phases flowing through a channel
Period: 19 Jun 2012
Nicolas Javier Alvarez (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Documents:
IMA6Temp_NickKerem_Three_layer_systems_Abstract.pdf
Related event
6th Conference of the International Marangoni Association: Interfacial Fluid Dynamics and Processes
18/06/2012 → 22/06/2012
Haifa, Israel
Activity: Talks and presentations › Conference presentations

49th Nordic Polymer Days 2012
Period: 29 May 2012 → 31 May 2012
Sindhu Vudayagiri (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Description
Surface and release properties of PDMS films, NPD, Oral presentation
Related event
49th Nordic Polymer Days 2012
29/05/2012 → 31/05/2012
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Novel applications of microbial transglutaminase as a biocatalyst for benign amide synthesis
Period: 18 May 2012
Maria Gundersen Deslauriers (Speaker)
Department of Chemical and Biochemical Engineering
Center for Process Engineering and Technology
Microbial Physiology and Genetics
Related event
12th Edition of PROTEO Annual Symposium
17/05/2012 → 18/05/2012
Sherbrooke, Canada
Activity: Talks and presentations › Conference presentations

Enzyme engineering for medical and biocatalytic applications
Period: 12 May 2012
Maria Gundersen Deslauriers (Speaker)
Department of Chemical and Biochemical Engineering
Center for Process Engineering and Technology
Related event
Departmental Biochemistry retreat: Department of Biochemistry, Université de Montréal
11/05/2012 → 12/05/2012
Saint-Sauveur, Quebec, Canada
Activity: Talks and presentations › Conference presentations

Biorefinery Öresund Conference 'Biorefining from raw material to high value products'
Period: 1 May 2012 → 30 Apr 2015
Peam Cheali (Speaker)
Krist V. Gernaey (Speaker)
Gürkan Sin (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Cost Estimation for Early-Stage Synthesis and Design of Biorefinery Networks
Period: 1 May 2012 → 30 Apr 2014
Peam Cheali (Other)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
The full author list is as follows: Peam Cheali, Krist V Gernaey, Gürkan Sin

Related event
2014 AIChE Annual Meeting: American Institute of Chemical Engineers
16/11/2014 → 21/11/2014
Atlanta, United States
Activity: Talks and presentations › Conference presentations

Synthesis and design of hybrid biorefinery systems – a structural optimisation approach and uncertainty analysis
Period: 1 May 2012 → 30 Apr 2015
Peam Cheali (Speaker)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
The full author list is as follows: Peam Cheali, Alberto Quaglia, Krist Gernaey, Gürkan Sin

Related event
21st International Congress of Chemical and Process Engineering
23/08/2014 → 27/08/2014
Prague, Czech Republic
Activity: Talks and presentations › Conference presentations

Uncertainty analysis in raw material and utility cost of biorefinery synthesis and design
Period: 1 May 2012 → 30 Apr 2015
Peam Cheali (Other)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Description
The full authors are as follows. Peam Cheali, Alberto Quaglia, Krist Gernaey, Gürkan Sin

Related event
24th European Symposium on Computer Aided Process Engineering
15/06/2014 → 18/06/2014
Budapest, Hungary
Activity: Talks and presentations › Conference presentations
Process engineering tools to guide implementation and scale-up of transaminase cascades
Period: 13 Apr 2012
Pär Tufvesson (Speaker)
Department of Chemical and Biochemical Engineering
Center for Process Engineering and Technology
Documents:
Abstract

Related event
Multistep Enzyme-Catalyzed Processes 2012
10/04/2012 → 13/04/2012
Graz, Austria
Activity: Talks and presentations › Conference presentations

Find the energy – the future is coming
Period: 19 Mar 2012 → 28 Mar 2012
Mette Sustmann Carter (Participant)
Department of Chemical and Biochemical Engineering
Ecosystems Programme

Description
Participation in five science theatre performances, 19-28 March, Roskilde, Holbæk, Slagelse, Nakskov and Vordingborg, DK.
Documents:
Avisomtale.pdf
Activity: Other

European Coating
Period: 14 Mar 2012
Kristian Petersen Nørgaard (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

Description
Oral presentation at European coatings conference - Fire retardant coatings in Berlin

Related event
European Coating: Fire Retardant Coatings
13/03/2012 → 14/03/2012
Berlin, Germany
Activity: Talks and presentations › Conference presentations

Kitasato University Hospital
Period: 2011
Marcel Tutor Ale (Visiting researcher)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Description
Bioassay of Fucoidan from Brown Seaweed

Anti-cancer activity assay and immune response of fucoidan by natural killer cells activity assay.
Activity: Visiting an external institution › Visiting another research institution
Microbial transglutaminase; exploration of substrate specificity, and biocatalytic applications
Period: 18 Nov 2011
Maria Gundersen Deslauriers (Speaker)
Department of Chemical and Biochemical Engineering
Center for Process Engineering and Technology

Related event
14th Chemistry and Biochemistry Graduate Research Conference: Concordia University
Montréal, Canada
Activity: Talks and presentations › Conference presentations

Post Combustion CCS activities at Center for Energy Resources Engineering: DTU Climate Centre Seminar on CCS
Period: 22 Sep 2011
Philip Loldrup Fosbøl (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Documents:
philip.pdf

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Student Info Meeting
Period: 1 Jun 2011
Marcel Tutor Ale (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Related event
Student Info Meeting
01/06/2011 → 01/06/2011
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Poly(ε-caprolactone) – a viable scaffold for design of intriguing nanobiomaterials: Lecture delivered at University Halle-Wittenberg, Germany
Period: 17 May 2011
Søren Hvilsted (Guest lecturer)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre
Documents:
Halle-Wittenberg_Abstract_17_May_2011.pdf

Related external organisation
University of Halle-Wittenberg
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

BIT’s 1st Annual Congress of Marine Biotechnology
Period: 25 Apr 2011 → 30 Apr 2011
Marcel Tutor Ale (Speaker)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

**Description**
Young Scientists' Forum: The Latest Research in Marine Biotechnology.

BIT's 1st Annual Congress of Marine Biotechnology (WCMB-2011), held in Dalian World Expo Center on April 25-30, 2011. With 350 participants from more than 30 countries.

**Related event**

**BIT's 1st Annual Congress of Marine Biotechnology**
25/04/2011 → 29/04/2011
Dalian, China
Activity: Talks and presentations › Conference presentations

**Building and sustaining an Industrial Consortium – The experience of DTU-CAPEC**
Period: 22 Apr 2011
Rafiqul Gani (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

**Related event**

**Building and sustaining an Industrial Consortium – The experience of DTU-CAPEC: UTM, Johar Bahru, Malaysia, 22 April**
22/04/2011 → 22/04/2011
Johar Bahru, Malaysia
Activity: Talks and presentations › Conference presentations

**Managing the Complexity in Product and Process Engineering**
Period: 17 Mar 2011
Rafiqul Gani (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

**Description**
Departmental Seminar

**Related external organisation**

**National Technical University of Athens**
Greece
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

**CAPEC Overview and Status - 2011**
Period: 10 Feb 2011
Rafiqul Gani (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

**Related event**

**CAPEC Overview and Status - 2011: Invited Seminar**
10/02/2011 → …
Lonza, Switzerland
Activity: Talks and presentations › Conference presentations
CAPEC Overview and Status - 2011
Period: 27 Jan 2011
Rafiqul Gani (Invited speaker)
Computer Aided Process Engineering Center
Department of Chemical and Biochemical Engineering

Related external organisation
DSM
Netherlands
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Oral presentation at the 25th European SYmposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia
Period: 1 Jan 2011 → …
Negar Sadegh (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Center for Energy Resources Engineering

Related event
Thermodynamic modeling of sour gas cleaning process with alkanolamines: ESAT
01/06/2011 → …
Saint Petersburg, Russian Federation
Activity: Talks and presentations › Conference presentations

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Oral presentation at the 25th European SYmposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia
Period: 1 Jan 2011 → …
Georgios Kontogeorgis (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Center for Energy Resources Engineering

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Negar Sadegh (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Center for Energy Resources Engineering

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations
Thermodynamic modeling of sour gas cleaning process with alkanolamine: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Georgios Kontogeorgis (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Center for Energy Resources Engineering

Period: 29 Aug 2010 → 3 Sep 2010
Muhammad Shafique Bashir (Speaker)
Department of Chemical and Biochemical Engineering
CHEC Research Centre

20th International Seaweed Symposium
Period: 22 Feb 2010 → 26 Feb 2010
Marcel Tutor Ale (Participant)
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering

Recent Advances in Fermentation Technology
Period: 8 Nov 2009 → 11 Nov 2009
Daniel Schäpper (Participant)
Department of Chemical and Biochemical Engineering

In the research and development phase of industrial fermentation processes, typically a tremendous research effort is put into both optimisation of the strain and the process conditions. This is often done in microtiter plates or by using shake-flask cultures as they are easy to set up. However, only batch experiments are possible and conditions are not well-controlled. This might result in deviations from results that would be obtained in industrial scale reactors. Bench-scale
reactor cultivations provide an alternative where conditions can be well-controlled and industrial conditions mimicked. However, this type of cultivations are rather labour intense and are therefore not a viable alternative when large number of strains or conditions should be screened. Microbioreactors offer the possibility to circumvent many of the above-mentioned problems: (1) Many parallel reactors allows for high-throughput screening; (2) The working volumes are very small, keeping costs low; (3) On-line measurements and control are possible (4) The reactors can be fabricated from polymers, thus making them disposable after use; (5) Finally, for batch type microbioreactors, the fermentation variables compare favourably with bench scale reactors, which indicates that the right culture physiology can be maintained at small vs. larger scale, making the technology commercially viable.

Place: San Diego, CA, USA

Related event

Recent Advances in Fermentation Technology 2009: RAFT 8
San Diego, United States
Activity: Attending an event › Participating in or organising a conference

Recent Advances in Fermentation Technology
Period: 8 Nov 2009 → 11 Nov 2009
Krist V. Gernaey (Participant)
Department of Chemical and Biochemical Engineering

Description
Disposable continuous culture microbioreactor with yeast for screening and process development applications (RAFT);
VIII: Given at: Recent Advances in Fermentation Technology (RAFT VIII)

In the research and development phase of industrial fermentation processes, typically a tremendous research effort is put into both optimisation of the strain and the process conditions. This is often done in microtiter plates or by using shake-flask cultures as they are easy to set up. However, only batch experiments are possible and conditions are not well-controlled. This might result in deviations from results that would be obtained in industrial scale reactors. Bench-scale reactor cultivations provide an alternative where conditions can be well-controlled and industrial conditions mimicked. However, this type of cultivations are rather labour intense and are therefore not a viable alternative when large number of strains or conditions should be screened. Microbioreactors offer the possibility to circumvent many of the above-mentioned problems: (1) Many parallel reactors allows for high-throughput screening; (2) The working volumes are very small, keeping costs low; (3) On-line measurements and control are possible (4) The reactors can be fabricated from polymers, thus making them disposable after use; (5) Finally, for batch type microbioreactors, the fermentation variables compare favourably with bench scale reactors, which indicates that the right culture physiology can be maintained at small vs. larger scale, making the technology commercially viable.

Place: San Diego, CA, USA

Related event

Recent Advances in Fermentation Technology 2009: RAFT 8
San Diego, United States
Activity: Attending an event › Participating in or organising a conference

4th STIPOMAT Conference
Period: 21 Sep 2008 → 24 Sep 2008
Anders Egede Daugaard (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Talk about "Functionalized conducting Polymers for Cell Processing" presented at 4th STIPOMAT Conference

Place: Lacanau, France

Related event

4th STIPOMAT Conference
21/09/2008 → 29/09/2008
Lacanau, France
4th STIPOMAT Conference
Period: 21 Sep 2008 → 24 Sep 2008
Søren Hvilsted (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Talk about "Functionalized conducting Polymers for Cell Processing" presented at 4th STIPOMAT Conference

Place: Lacanau, France

Related event

4th STIPOMAT Conference
21/09/2008 → 29/09/2008
Lacanau, France
Activity: Attending an event › Participating in or organising a conference

Ionic Liquids: From Knowledge to Application
Martin Etchells Vigild (Participant)
The Danish Polymer Centre
Department of Chemical and Biochemical Engineering

Description
Hydrophilic Nanoporous Polystyrenes and 1,2 - Polybutadiene via Surface-initiated Atom Transfer Radical Polymerization

Place: American Chemical Society 236th National Meeting. Philadelphia, Pennsylvania, USA
Degree of recognition: International

Related event

Ionic Liquids: From Knowledge to Application: 236th ACS National Meeting
17/08/2008 → 21/08/2008
Philadelphia, (PA), United States
Activity: Attending an event › Participating in or organising a conference

Nordic Polymer Days 2008
Period: 11 Jun 2008 → 13 Jun 2008
Katja Jankova Atanasova (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Talk about "Hydrophilic Nanoporous Polystyrenes and 1,2 - Polybutadienes" presented at Nordic Polymer Days NPD 2008, June 11-13

Place: Stockholm, Sweden

Related event

Nordic Polymer Days 2008
11/06/2008 → 13/06/2008
Stockholm, Sweden
Activity: Attending an event › Participating in or organising a conference
Nordic Polymer Days 2008
Period: 11 Jun 2008
Martin Etchells Vigild (Participant)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Talk about "Hydrophilic Nanoporous Polystyrenes and 1,2 - Polybutadienes" presented at Nordic Polymer Days NPD 2008, June 11-13

Place: Stockholm, Sweden

Related event
Nordic Polymer Days 2008
11/06/2008 → 13/06/2008
Stockholm, Sweden
Activity: Attending an event › Participating in or organising a conference

Ionic Liquids: From Knowledge to Application
Period: 1 Jan 2008 → …
Katja Jankova Atanasova (Participant)
The Danish Polymer Centre
Department of Chemical and Biochemical Engineering

Description
Hydrophilic Nanoporous Polystyrenes and 1,2 - Polybutadiene via Surface-initiated Atom Transfer Radical Polymerization

Place: American Chemical Society 236th National Meeting. Philadelphia, Pennsylvania, USA
Degree of recognition: International

Related event
Ionic Liquids: From Knowledge to Application: 236th ACS National Meeting
17/08/2008 → 21/08/2008
Philadelphia, (PA), United States
Activity: Attending an event › Participating in or organising a conference

Talk about "Hydrophilic Nanoporous Polystyrenes and 1,2 - Polybutadienes" presented at Nordic Polymer Days NPD 2008, June 11-13
Period: 1 Jan 2008 → …
Fengxiao Guo (Speaker)
Department of Chemical and Biochemical Engineering
The Danish Polymer Centre

Description
Place: Stockholm, Sweden

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Prizes:

Best Oral Presentation Award
Seyed Soheil Mansouri (Recipient)
Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Description
9th IFAC Symposium on Advanced Control of Chemical Processes ADCHEM 2015 – Whistler, Canada, 7–10 June, 2015

Details
Awarded date: 7 Jun 2015
Degree of recognition: International
Prize: Prizes, scholarships, distinctions

Best Presentation
Seyed Soheil Mansouri (Recipient)
Department of Chemical and Biochemical Engineering, CAPEC-PROCESS

Description
2015 Annual AIChE Meeting in Salt Lake City

Details
Awarded date: 10 Nov 2015
Granting Organisations: American Institute of Chemical Engineers
Prize: Prizes, scholarships, distinctions

Press clippings:

Lad Autopiloten overtage fyringen i brændeovnen
Jytte Boll Illerup
05/12/2014
CHEC Research Centre, Department of Chemical and Biochemical Engineering

Media coverage (1)

Lad Autopiloten overtage fyringen i brændeovnen
05/12/2014
Dynamo, Denmark
Marianne Vang Ryde
http://www.dtu.dk/Nyheder/2014/12/Dynamo-Lad-autopiloten-overtage-fyringen-i-braendeovnen
Jytte Boll Illerup
Press / Media

Sådan kan intelligent materiale bruges som kunstige muskler
Frederikke Bahrt Madsen
10/09/2013
The Danish Polymer Centre, Department of Chemical and Biochemical Engineering

Media contribution (1)

Sådan kan intelligent materiale bruges som kunstige muskler
10/09/2013
Videnskab.dk, Web
http://91.102.88.126/teknologi/sadan-kan-intelligent-materiale-bruges-som-kunstige-muskler
Frederikke Bahrt Madsen
Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Press / Media

Dielektriske elektroaktive polymerer
Frederikke Bahrt Madsen
03/09/2013
The Danish Polymer Centre, Department of Chemical and Biochemical Engineering

Media contribution (1)

Dielektriske elektroaktive polymerer
03/09/2013
P1, Radio
http://podcast.dr.dk/P1/videnskabens_verden/2013/videnskabens_verden_1309031403.mp3