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.
In this study a CO$_2$ 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%, CO$_2$ partial pressures up to 50 kPa, solvent loading between 0 and 0.5 mole CO$_2$ 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, CO$_2$ partial pressure) of the different process conditions on the mass transfer, whereas the SP model is limited to applications with low CO$_2$ 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.
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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- BFI (2017): BFI-level 1
- 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
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- ISI indexed (2013): ISI indexed yes
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- 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
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.292 SNIP 1.846 CiteScore 3.03
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.372 SNIP 1.75
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.339 SNIP 1.797
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
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 Catalysis y Petroleoquimica, Rey Juan Carlos University, 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)
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Journal: Chemical Engineering Journal
Volume: 335
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BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Flow characterization of aerated bubble column reactor using electrical resistance tomography and computational fluid dynamic methods

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Ryerson University
Authors: Bach, C. (Intern), Albæk, M. O. (Intern), Krühne, U. (Intern), Gernaey, K. V. (Intern), Ein-Mozaffari, F. (Ekstern)
Number of pages: 1
Publication date: 2018
Event: Abstract from 10th World Congress of Chemical Engineering (WCCE10), Barcelona, Spain.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Journal article – Annual report year: 2018

High-Order Approximation of Chromatographic Models using a Nodal Discontinuous Galerkin Approach
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.
Large scale simulations of Trichoderma reesei fermentation using computational fluid dynamics: Approach and early successes

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Novozymes A/S
Authors: Bach, C. (Intern), Albæk, M. O. (Ekstern), Krühne, U. (Intern), Gernaey, K. V. (Intern)
Number of pages: 1
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Event: Abstract from Recent Advances in Fermentation Technology (RAFT 2017), Florida, United States.
Main Research Area: Technical/natural sciences
Publication: Research › Conference abstract for conference – Annual report year: 2018

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, devices 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
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Main Research Area: Technical/natural sciences
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Publication information
Journal: Sensors and Actuators B: Chemical
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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
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Main Research Area: Technical/natural sciences

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Multiscale Modeling of Poly(lactic acid) Production: From Reaction Conditions to Rheology of Polymer Melt
Abstract Poly(L-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)
Pages: 361–375
Publication date: 2018
Main Research Area: Technical/natural sciences

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Journal: Chemical Engineering Journal
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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
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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**
State: Published
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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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
Scopus rating (2007): SJR 2.014 SNIP 0.992
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.
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
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Chulalongkorn University
Authors: Anantasarn, N. (Ekstern), Suriyapraphadilok, U. (Ekstern), Babi, D. K. (Intern)
Pages: 56-73
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BFI (2017): BFI-level 2
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Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
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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
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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
Web of Science (2006): Indexed yes
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
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.042 SNIP 0.92
Web of Science (2002): Indexed yes
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, 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)
Pages: 2222-2226
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Conference: 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 01/10/2017 - 01/10/2017
Lactic acid bacteria, Parameter estimation, Sensitivity analysis, Identifiability analysis, uncertainty analysis mathematical and computer techniques
DOIs: 10.1016/B978-0-444-63965-3.50372-X
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

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.

**General information**
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Inbicon A/S, University of Copenhagen
- **Authors:** Bisgaard, T. (Intern), Mauricio Iglesias, M. (Intern), Huusom, J. K. (Intern), Gernaey, K. V. (Intern), Dohrup, J. (Ekstern), Petersen, M. A. (Ekstern), Abildskov, J. (Intern)
- **Pages:** 5692-5704
- **Publication date:** 2017
- **Main Research Area:** Technical/natural sciences

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- **Volume:** 56
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  - BFI (2017): BFI-level 2
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 2
  - Web of Science (2016): Indexed yes
  - 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
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 (ΔAnatg8) 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.
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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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
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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
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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BFI (2017): BFI-level 2
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BFI (2016): BFI-level 2
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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
Analysis and Modelling of an Industrial Pressure Filtration using Process Data

In order to understand a series of pressure leaf filters located in the downstreamline 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
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, CP Kelco ApS
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Pages: 12643-12648
Publication date: 2017
An Efficient Experimental Design Strategy for Modelling and Characterization of Processes

Designing robust, efficient and economic processes is a main challenge for the biotech industries. To achieve a well-designed bioprocess, understanding the ongoing phenomena and the involved reaction kinetics is crucial. By development of advanced miniaturized reactors, a promising opportunity arises for parallel screening of multiple processes in reduced volumes within high throughput platforms. However, the level of accessible information from each set of experimental design remains to be one of the main issues particularly in the case of complex biosystems. This work introduces a novel generic Model-based Design of Experiments (M-DoE) routine with its main target being model development and system characterization. With the new M-DoE strategy, an improved set of informative experiments are suggested, which consequently reduces the demand for physical resources and analysis. The routine proposes a set of optimum experimental settings to support structural model definition, kinetic order estimation and parameter estimation during a model building procedure and process characterization.

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.
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.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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BFI (2018): BFI-level 2
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
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.
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.

**General information**

State: Published
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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
Scopus rating (2007): SJR 1.347 SNIP 1.523
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.308 SNIP 1.553
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.445 SNIP 1.801
Scopus rating (2004): SJR 1.301 SNIP 1.858
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 (550 L) 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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, LEO Pharma AS, Novozymes AS, Novozymes
Authors: Mears, L. (Intern), Stocks, S. M. (Ekstern), Albaek, M. O. (Ekstern), Cassells, B. (Ekstern), Sin, G. (Intern), Gernaey, K. (Intern)
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 4.14 SJR 1.411 SNIP 1.163
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre
Authors: Frauzem, R. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
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Application of a Mechanistic Model as a Tool for On-line Monitoring of Pilot Scale Filamentous Fungal Fermentation Processes - The Importance of Evaporation Effects: Mechanistic model for pilot scale monitoring
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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering, Novozymes AS
Authors: Mears, L. (Intern), Stocks, S. M. (Ekstern), Albæk, M. O. (Ekstern), Sin, G. (Intern), Gernaey, K. V. (Intern)
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Main Research Area: Technical/natural sciences

Publication information
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.

General information
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Scopus rating (2016): CiteScore 2.12 SJR 0.668 SNIP 0.762
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.727 SNIP 0.825 CiteScore 2.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.808 SNIP 0.931 CiteScore 2.2
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
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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium, King Mongkut's Institute of Technology Ladkrabang
Authors: Papadakis, E. (Intern), Anantpinijwatna, A. (Ekstern), Woodley, J. (Intern), Gani, R. (Intern)
Number of pages: 25
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
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.

**General information**

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Vegetable oils, Fatty acids, Kinetic modeling, Uncertainty analysis
DOI: 10.1016/B978-0-444-63965-3.50198-7

**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.

**General information**

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Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Environmental Chemistry, Water Resources Engineering
Authors: Ramin, P. (Intern), Valverde Pérez, B. (Intern), Polesel, F. (Intern), Locatelli, L. (Intern), Plósz, B. G. (Intern)
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**Publication information**

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Article number: 9390
ISSN (Print): 2045-2322
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BFI (2018): BFI-level 1
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.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
Authors: Ringborg, R. H. (Intern), Pedersen, A. T. (Intern), Woodley, J. (Intern)
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Scopus rating (2016): CiteScore 4.33 SJR 1.636 SNIP 0.932
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.

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Authors: Woodley, J. (Intern)
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Web of Science (2015): Indexed yes
Biocatalysis, Bioprocess, Fermentation, Metabolic engineering, Process intensification, Protein engineering

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.

**Calibration of the comprehensive NDHA-N₂O 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.
Calibration of the NDHA N2O model via respirometric assays

General information
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Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Centre for oil and gas – DTU, 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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Main Research Area: Technical/natural sciences
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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
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark, SpinChem AB
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Web of Science (2016): Indexed yes
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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
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.
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.
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, \( k_La \), was estimated to be \( 344 \text{ h}^{-1} \) in the \( 100 \text{ mL} \) ACR, opposed to only \( 104 \text{ h}^{-1} \) 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.
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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Frutiger, J. (Intern), Cignitti, S. (Intern), Abildskov, J. (Intern), Woodley, J. (Intern), Sin, G. (Intern)
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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
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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), Albaek, M. O. (Ekstern), Gernaey, K. V. (Intern), Krühne, U. (Intern)
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Computational_Fluid_Dynamics_En_genvej_til_procesindsigt.pdf
Publication: Communication › Journal article – Annual report year: 2017

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
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Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre, Technical University of Denmark, Politecnico di Milano
Authors: Rosengarta, A. (Ekstern), Bertran, M. (Intern), Manenti, F. (Ekstern), Citterio, A. (Ekstern), Woodley, J. (Intern), Gani, R. (Intern)
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Volume: 40
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Editors: Espuña, A., Graells, M., Puigjaner, L.
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.

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.
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.
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.

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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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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
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Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
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Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
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Scopus rating (2010): SJR 0.433 SNIP 0.957
Web of Science (2009): Indexed yes
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Design_and_simulation_of_rate_based_co2.pdf
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**Design of a gas-inducing impeller using Computational Fluid Dynamics**

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Technical University of Denmark, BIO-AQUA
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.
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 gMPPA·L⁻¹, a purity up to 70% 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.
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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Technical University of Denmark
Authors: Nielsen, R. F. (Ekstern), Huusom, J. K. (Intern), Abildskov, J. (Intern)
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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
Dynamic modelling of pectin extraction describing yield and functional characteristics

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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CP Kelco ApS, University of Copenhagen, National Polytechnic Institute of Chemical and Industrial Engineering and Technology
Authors: Andersen, N. M. (Intern), Cognet, T. (Ekstern), Santacoloma, P. A. (Ekstern), Larsen, J. (Ekstern), Armagan, I. (Ekstern), Larsen, F. H. (Ekstern), Gernaey, K. (Intern), Abildskov, J. (Intern), Huusom, J. K. (Intern)
Pages: 61-71
Publication date: 2017
Main Research Area: Technical/natural sciences
Degree of esterification, Dynamic modelling, Intrinsic viscosity, Pectin extraction, Yield, Dynamic models
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.

General information
State: Published
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)
Pages: 1759-1764
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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Publisher: Elsevier Science
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Volume: 40
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
U-Loop Reactor, Single Cell Protein, Optimization, Optimal Control
DOIs: 10.1016/B978-0-444-63965-3.50295-6
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

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

Publication information
Journal: Catalysts
Volume: 7
Issue number: 8
Article number: 227
ISSN (Print): 2073-4344
Ratings:
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
State: Published
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.
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.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, CAPEC-PROCESS, CHEC Research Centre, KT Consortium, Center for BioProcess Engineering
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Main Research Area: Technical/natural sciences

**Publication Information**

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Volume: 332
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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
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 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2001): Indexed yes
Original language: English

Microfluidics, Thiol-ene chemistry, Enzyme immobilization, Surface functionalization, Computational fluid dynamic simulation (CFD)
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 View the MathML source. $T_s$ was identified as most influential parameter on both $T_i$ and View the MathML source, followed by $P_c$ and the dried product mass transfer resistance $\alpha_R p$ for $T_i$ and View the MathML source, respectively. The GSA findings were experimentally validated for View the MathML source 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
State: Accepted/In press
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)
Number of pages: 16
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: European Journal of Pharmaceutics and Biopharmaceutics
ISSN (Print): 0939-6411
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.49 SJR 1.366 SNIP 1.409
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.414 SNIP 1.496 CiteScore 4.37
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.469 SNIP 1.586 CiteScore 4.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.558 SNIP 1.706 CiteScore 4.64
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.976 SNIP 1.933 CiteScore 5.15
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.794 SNIP 1.887 CiteScore 4.77
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.948 SNIP 1.933
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:
O.3.9.3_High_Temperature_Heat_Pump_Integration_using_Zeotropic_Working_F....pdf

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

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), Glanville, 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

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
Publication date: 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
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)
Number of pages: 15
Publication date: 2017

Host publication information
Title of host publication: Proceedings of ECOS 2017: 30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
Main Research Area: Technical/natural sciences
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Heat pump, Zeotropic mixture, Temperature glide, Exergy efficiency
Electronic versions:

Relations
Projects:
Improving efficiency of heat pumps by use of zeotropic mixtures for different temperature glides
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

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
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: the primary amine monoethanolamine (MEA), the sterically hindered primary amine 2-amino-2-methyl-1-propanol (AMP), the tertiary amine N-methyl-diestanolamine (MDEA) and the carbonate salt solution K₂CO₃ 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 K₂CO₃; 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 K₂CO₃ 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 K₂CO₃ at 313 K. Temperature and concentration did increase the enzymatic rate constant slightly in the
concentration range of 5–15 wt% K₂CO₃ 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.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS
Authors: Gladis, A. (Intern), Deslauriers, M. G. (Intern), Fosbøl, P. L. (Intern), Woodley, J. (Intern), von Solms, N. (Intern)
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Main Research Area: Technical/natural sciences

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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
Web of Science (2007): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2001): Indexed yes
Original language: English
Carbon capture, Carbonic anhydrase, Kinetics, Mass transfer, Solvent, Wetted wall column

**DOIs:**
10.1016/j.cej.2016.10.056
Source: FindIt
Source-ID: 2347626564
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Cignitti, S. (Intern), Woodley, J. (Intern), Abildskov, J. (Intern)
Number of pages: 6
Publication date: 2017

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Publisher: Elsevier Science
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Edition: 1
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Conference: 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 01/10/2017 - 01/10/2017
Waste heat, CAMD, Optimization, Product-process, Refrigerant, Refrigeration

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 1.2MW 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-dimethylpent-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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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.

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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.

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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.

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- Web of Science (2003): Indexed yes
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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 the 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 combining 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 endeavours. 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 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.

General information
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.
Modeling Electron Competition among Nitrogen Oxides Reduction and N$_2$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$_2$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$_2$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$_2$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$_2$O accumulation would not be intensified under hydrogen limiting conditions, due to the higher electron competition capacity of N$_2$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$_2$O accumulation.
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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 legislative. 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 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.

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Modelling and Validating a Deoiling Hydrocyclone for Fault Diagnosis using Multilevel Flow Modeling

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, requiring rigorous and reliable model building and testing. Multilevel Flow Modeling is a qualitative methodology 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.
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 (Xaa, Xsu, 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.
Modelling biotransformation of drug biomarkers by sewer biofilms

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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
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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.

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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.

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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.

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 MNCO2/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 enzymes, 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.
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 multiplant 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.
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.
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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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 (N2O+N2) 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.

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Web of Science (2015): Indexed yes
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Web of Science (2014): Indexed yes
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Scopus rating (2013): CiteScore 3.03
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BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.15
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 requires 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.
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
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Haldor Topsoe AS
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Main Research Area: Technical/natural sciences
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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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 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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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-phasic (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 (XTSS) control strategy (A1) better adapts the system to influent dynamics, improves phosphate (SPO4) accumulation by phosphorus accumulating organisms (XPAO) (41%), increases nitrification/denitrification efficiency (18%) and reduces aeration energy (Eaeration) (21%). The addition of iron [Formula: see text] for chemical P removal (A2) promotes the formation of ferric oxides (XHFO-H, XHFO-L, co-precipitation (XHFO-H,P,old and XHFO-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 (GH2s) reduced (36%) due to iron sulfide (XFeS) precipitation. As a consequence, there is also a slightly higher energy production (Eproduction) 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 (XMgNH4PO4) recovery ranging from 69 to 227 kg.day-1 depending on: (1) airflow (Qstripping); and, (2) magnesium (QMg(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.

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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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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.

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.
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.
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.
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.
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)
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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 $K_m$ values deviated by a factor of up to four from the thermodynamic equilibrium constant $K_{th}$. The observed concentration dependency of the experimental $K_m$ 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 ± 2.8 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.
Reliable Correlation for Liquid-Liquid Equilibria Outside the Critical Region

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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Virginia
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Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
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Removal of benzaldehyde from a water/ethanol mixture by applying scavenging techniques

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.
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
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, University of Virginia
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BFI (2014): BFI-level 1
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ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
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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
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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)
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Ressourcegenvinding – vejen til øget bæredygtighed i biobaserede produktionsprocesser


General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, BioProcess ApS
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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 units 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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Novozymes A/S
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.
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
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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.
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
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre
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Scopus rating (2007): SJR 0.126 SNIP 0.065
Scopus rating (2006): SJR 0.101 SNIP 0.005
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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 multiplant 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
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
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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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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
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Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
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BFI (2009): BFI-level 2
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Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
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Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241

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.

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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
Authors: Cignitti, S. (Intern), Mansouri, S. S. (Intern), Woodley, J. M. (Intern), Abildskov, J. (Intern)
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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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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
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)
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 metanotrophic 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.

Ultrasonic-assisted production of biodiesel FAME from rapeseed oil in a novel two-compartment reactor

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
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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 alkylation of isobutybenzene to 4-isobutylyphenylacetophenone, its further hydrogenation to IBPE (1,4-isobutylyphenylethanol) 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 irritations. 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**
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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 anorganic 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, though it 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.

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Uncertainty Assessment 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 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 temperatures 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 nitrites are building up. Oxygen availability should be regulated according to the measured controlled variable.
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.

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.

General information

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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 (Nmethyl-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.
Using MFM methodology to generate and define major accident scenarios for quantitative risk assessment studies

Generating and defining Major Accident Scenarios (MAS) are commonly agreed as the key step for quantitative risk assessment (QRA). The aim of the study is to explore the feasibility of using Multilevel Flow Modeling (MFM) methodology to formulating MAS. Traditionally this is usually done based on historical incidents or the outcome of HAZOP/HAZID. This paper suggests using MFM to model the plant, and then performs systematic reasoning based on the model to produce casual paths of plant failure scenarios. The cause trees generated by MFM are transformed into fault trees, which are then used to calculate likelihood of each MAS. Combining the likelihood of each scenario with a qualitative risk matrix, each major accident scenario is thereby ranked for consideration for detailed consequence analysis. The methodology is successfully highlighted using part of BMA-process for production of hydrogen cyanide as case study.

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
A useful complementary biomonitoring tool to study population-wide exposure to pesticides.

**General information**

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**Organisations:** Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Istituto di Ricerche Farmacologiche Mario Negri, University Jaume I, Norwegian Institute for Water Research, University of Bath, KWR Watercycle Research Institute, University of Antwerp, Swiss Federal Institute of Aquatic Science and Technology (Eawag)

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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 α-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.

General information
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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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Scopus rating (2008): SJR 0.556 SNIP 0.859
Web of Science (2008): Indexed yes
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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.

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 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. 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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 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. 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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 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.

General information

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ISI indexed (2013): ISI indexed yes
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.
A Generic Methodology for Superstructure Optimization of Different Processing Networks

In this paper, we propose a generic computer-aided methodology for synthesis of different processing networks using superstructure optimization. The methodology can handle different network optimization problems of various application fields. It integrates databases with a common data architecture, a generic model to represent the processing steps, and appropriate optimization tools. A special software interface has been created to automate the steps in the methodology workflow, allow the transfer of data between tools and obtain the mathematical representation of the problem as required by the optimization tool. The methodology and its implementation have been tested through various case studies.

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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 automatically created. This input file contains values of all the parameters of the generic process model. Then, the problem is solved in GAMS and the interface shows the results and allows for the selection of alternatives. The output from the synthesis stage (the first stage) is the optimal processing route for the defined problem and scenario, which can be transferred to a rigorous process simulator for the second stage (design stage). Here, the selected route needs to be further designed, simulated and analyzed. Then, more sustainable innovative designs can be developed in the third stage based on the output design from the second stage. This generic methodology and software interface can be applied to an array of problems within synthesis of processing networks. This is illustrated through case studies from two applications: the synthesis of biorefinery networks and the synthesis of sustainable carbon dioxide utilization processes.
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.

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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.
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.
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.

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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.

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A methodology for the sustainable design and implementation strategy of CO$_2$ utilization processes

This work presents a systematic methodology that has been developed for the design of sustainable CO$_2$ utilization processes that can mitigate CO$_2$ 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$_2$ 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$_2$ when cheap H$_2$ feeds are available.

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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
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Scopus rating (2013): SJR 0.759 SNIP 0.379 CiteScore 1.7
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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
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Journal: Fluid Phase Equilibria
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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
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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
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

General information
State: Published
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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.

**Application of e-KT-UNIFAC Model for Improved and Innovative Design of Biphasic Reacting Systems**

State: Published
Organizations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana, Korea University
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Number of pages: 1
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Main Research Area: Technical/natural sciences
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Source-ID: 124927828
Publication: Research › Conference abstract for conference – Annual report year: 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.
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.
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 prochiral 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.

General information
State: Published
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Pages: 602-608
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Main Research Area: Technical/natural sciences

Publication information
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.

General information
State: Published
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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 1.681 SNIP 2.477 CiteScore 4.6
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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.644 SNIP 2.581 CiteScore 4.47
ISI indexed (2013): 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
Scopus rating (2010): SJR 1.419 SNIP 1.742
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 reactor. A benchmark dispersion axial model displaying different temperature profiles is used to illustrate our findings.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Veracruzana, Universidad Autonoma Metropolitana
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Publication date: 2016
Main Research Area: Technical/natural sciences

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Web of Science (2016): Indexed yes
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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.
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 brazzena 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.
Bioinspired Multifunctional Membrane for Aquatic Micropollutants Removal

Micropollutants present in water have many detrimental effects on the ecosystem. Membrane technology plays an important role in the removal of micropollutants, 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 micropollutants.
Bioprocess Development of (R)-Perillic Acid Production with a Whole-Cell Biocatalyst

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, BRAIN AG
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Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

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 (m² 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 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

General information
Catchment & sewer network simulation model to benchmark control strategies within urban wastewater systems

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.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University, University of Exeter
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Main Research Area: Technical/natural sciences
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.
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 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.

Continuous production of chitooligosaccharides by an immobilized enzyme in a dual-reactor system

A chitosanolytic activity found in a commercial α-amylase from Bacillus amylolyquefaciens (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⁻¹ h⁻¹, with a conversion yield of 73%. In contrast, at the highest dilution rate, the productivity was nearly 200 gCOS L⁻¹ h⁻¹, but the conversion yield dropped to around 40%.

General information
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Control of wastewater N2O 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 N2O 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 N2O 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 N2O emitted (approximately 35%). On the other side, this reduction of N2O 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 N2O 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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering
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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 greenmicro-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.
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.

General information
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ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.887 SNIP 0.896
Web of Science (2010): Indexed yes
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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
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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 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.
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.

General information
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Web of Science (2015): Indexed yes
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Scopus rating (2013): SJR 0.901 SNIP 1.875 CiteScore 2.64
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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
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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. Smidth A/S
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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 digester 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
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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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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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 MMS/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 MonteCarlo 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 forchemicals and fuels.

General information
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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 non-profitable (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.
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Web of Science (2012): Indexed yes
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
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Scopus rating (2009): SJR 1.002 SNIP 1.164
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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.

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 proved 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 (foreexample, 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 products). 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 a 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.

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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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Groningen, BASF
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Publication information
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.
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
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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.


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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Haldor Topsoe AS
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Forbedring af industrielle processers 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.

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Novozymes A/S, Swiss Federal Institute of Aquatic Science and Technology, Technical University of Denmark
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Forbedring af industrielle processers 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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- Web of Science (2016): Indexed yes
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- Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
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- 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
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- Web of Science (2009): Indexed yes
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- 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
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.309 SNIP 1.64
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.297 SNIP 1.654
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 1.694 SNIP 1.578
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 1.749 SNIP 1.725
- Web of Science (2002): Indexed yes
- Scopus rating (2001): SJR 2.16 SNIP 2.077
- Web of Science (2001): Indexed yes
**Fundamentals of process intensification: A process systems engineering view**

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.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Babi, D. K. (Intern), Sales Cruz, A. M. (Intern), Gani, R. (Intern)
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**Generation of synthetic influent data to perform (micro)pollutant wastewater treatment modelling studies**

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 influence 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.

**General information**
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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium
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Main Research Area: Technical/natural sciences

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. Therewith, it should be possible to gradually reach improved culture efficiency as defined in the objective function.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Sharif University of Technology
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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.

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Group-Contribution based Property Estimation and Uncertainty analysis for Flammability-related Properties

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.

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Scopus rating (2011): SJR 1.918 SNIP 2.11 CiteScore 4.81
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Scopus rating (2010): SJR 1.671 SNIP 1.704
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
Example application of the models are shown for a selected class of chemicals to highlight the application range of models.

**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-allylcarkinol") to give a mixture of cis- and trans-9H-thioxanthene, 2-chloro-9-(2-propenylidene)-(9CI) ("N746-budadienes"). 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.

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).

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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 (W_A and W_B). 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 W_{HK} and W_{LH}). 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 is 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.

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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.
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.

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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).

Conclusion: We established the measurement of oxygen transfer rates from air into these organic solvents. Furthermore, the feasibility of online oxygen measurements in organic solvents has also been demonstrated, paving the way for new opportunities in process control.
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 online process control and optimization.

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 the each cell. Experiments are performed on red blood cells (RBCs), peripheral blood lymphocytes (PBLs) and myelogenous leukemia tumor cells (K562).
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.

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Model-Based Monitoring of an Industrial Batch Pectin Extraction

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Number of pages: 1
Publication date: 2016
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.
Modelling and control of nitrogen and phosphorus removing systems

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Modelling and sensitivity analysis of urinary platinum excretion in anticancer chemotherapy for the recovery of platinum

Platinum (Pt) based antineoplasticss 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 antineoplasticss 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.

General information
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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.
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.
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

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Pages: 1720-1730
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.

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NLP modeling for the optimization of LiBr-H$_2$O 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-H$_2$O 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. Around three-quarters of the minimal total annual cost correspond to capital expenditures and the rest to operating expenditures. The generator and evaporator represent together around 70% of the capital expenditures. The absorber is the largest contributor to both the total heat transfer area and the total exergy loss rate, with around 33.19 and 39.16%, respectively, when the total annual cost is minimized.

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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 engineering 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.
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) tetrabenzoporphyrin (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.
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 into 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 considerable 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 10 K. 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.

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Optimal algal cultivation for used water resource recovery

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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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Phase Equilibria Prediction for Systems Containing Lipids

In recent years, utilization of fats and oils has started to shift towards the bioindustrymakingthem 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 largescaleindustry [1]. Such developments have led to new challenges regarding the design and development of better performing processes and products. Despite the advances in propertymodelling and process design techniques available via different computeraidedmethods 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 qualitiy 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 (vapourliquid equilibrium VLE, solidliquid 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 OriginalUNIFAC 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).
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 N₂O emitted from WWT 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 N₂O emissions. However, in full-scale continuously-aerated wastewater treatment systems such control strategies cannot be implemented. Furthermore, the available control strategies developed for N₂O 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 N₂O emission minimization is developed. More specifically, the control strategy is designed in order to prevent the typical biological mechanisms triggering N₂O 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 N₂O emissions but also the effluent quality and the operational costs, is carried out. This is because the reduction of the carbon footprint of WWT plants cannot be achieved at the expense of worse effluent quality and unreasonably-high operational costs. To build simulation environments where N₂O controller could be benchmarked against a reference scenario, three different benchmark simulation models are developed by including N₂O-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 N₂O predictions by the three models. Since there is at the moment no consensus model considered to describe reliably N₂O emissions from WWT plants, all the three models are used for testing the N₂O 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 N₂O 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 N₂O 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 N₂O 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, N₂O 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 N₂O 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.
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.
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.

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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.
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 aquaeolei 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.

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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 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.
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 obtain 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.

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**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 experiments 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 make the product design 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 (VPPD-Lab) 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) creation of 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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Main Research Area: Technical/natural sciences
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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

Quantifying the importance of flow maldistribution in numbered-up microreactors
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 an acertain 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 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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Ghent University
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DOIs:
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
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Electronic versions: Rational_and_Evolutionary_Engineering.pdf

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Poster and rapid fire presentation
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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
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BFI (2017): BFI-level 1
Scopus rating (2016): CiteScore 3.83 SJR 0.844 SNIP 1.355
Web of Science (2016): Indexed yes
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Scopus rating (2014): SJR 0.596 SNIP 1.086 CiteScore 2.21
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Activated sludge, ASM1 model, Batch bioreactor, Dynamics, Model reduction, Reaction invariant
DOIs:
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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
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Pages: 9865-9872
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BFI (2017): BFI-level 2
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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
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
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. 3-8).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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Electronic versions:
Safeprops_Mark_AIChE2016.pdf
Links:
https://aiche.confex.com/aiche/2016/webprogram/Paper466860.html
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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/wo) 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
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.

General information
State: Published
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Number of pages: 1
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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**
State: Published
Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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Number of pages: 1
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Event: Poster session presented at 5th IWA/WEF Wastewater Treatment Modelling Seminar 2016, Annecy, France.
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Modelling, N2O, Uncertainty, Production pathway, Experimental design
Electronic versions:
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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.

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Conference: 26th European Symposium on Computer-Aided Process Engineering, Portorož, Slovenia, 12/06/2016 - 12/06/2016
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2016
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.
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. It is formulated based on engineering knowledge and is coupled to process models developed in Aspen and Matlab, together with multi-objective optimization 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.

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) $H_\infty$ 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 $H_\infty$ 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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Organisations: Department of Chemical and Biochemical Engineering, Department of Environmental Engineering, Water Technologies, CAPEC-PROCESS
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.41 SJR 1.21 SNIP 2.241
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.338 SNIP 2.028 CiteScore 3.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.521 SNIP 2.735 CiteScore 3.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
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
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.316 SNIP 2.59 CiteScore 2.9
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.305 SNIP 2.203
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.282 SNIP 2.772
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.458 SNIP 2.698
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.425 SNIP 2.086
Scopus rating (2006): SJR 1.739 SNIP 2.369
Scopus rating (2005): SJR 1.016 SNIP 2.362
Scopus rating (2004): SJR 1.019 SNIP 1.824
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.

General information
State: Published
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 2
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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
Systematic design of optimal control systems for WWTPs: case study of the SHARON-Anammox process

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Organisations: Department of Environmental Engineering, Water Technologies, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Valverde Perez, B. (Intern), Mauricio Iglesias, M. (Intern), Sin, G. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at 5th IWA/WEF Wastewater Treatment Modelling Seminar 2016, Annecy, France.
Main Research Area: Technical/natural sciences
Electronic versions: WWTmod2016_SA_MIM.pdf
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 hence 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.
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.
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.

General information
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Pages: 348–364
Publication date: 2016
Systematic methods and tools for design of sustainable chemical processes for CO₂ 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 CO₂ 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.
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 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

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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 of 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.

General information
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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.

General information
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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 straightforward 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 in 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 C₁ 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 keys 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.

General information
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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
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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
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.

General information
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Web of Science (2016): Indexed yes
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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
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
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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/expanded 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.
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. Penge 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
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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
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.998 SNIP 2.25 CiteScore 4.25
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 stand-alone 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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of KwaZulu-Natal, University of Cape Town, University of Queensland, Lund University
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.

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.
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: nitrification, nitratification, 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.

General information
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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.

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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.

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_{cryst}) and, for calcite, have a 2nd order dependency (exponent n ¼ 2.05 ± 0.29) on thermodynamic supersaturation (s). Parameter analysis indicated that the model was more tolerant to a fast kinetic coefficient (k_{cryst}) and so, in general, it is recommended that a large k_{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_{cryst}. The influence of magnesium (a common and representative added impurity) on k_{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
with n = 2 (or n = 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  
**Organisations:** Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Queensland  
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- BFI (2011): BFI-level 2  
- Scopus rating (2011): SJR 2.867 SNIP 2.374 CiteScore 5.43  
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- BFI (2010): BFI-level 2  
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- Web of Science (2007): Indexed yes  
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- Web of Science (2006): Indexed yes  
- Scopus rating (2005): SJR 2.114 SNIP 2.337  
- Web of Science (2005): Indexed yes
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.

General information
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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 e MI(N)LP e 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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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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Journal: Environmental Modelling & Software
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.

**General information**

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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 syst-tem operation. However, for the actual design of control systems urban drain-age 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 planner and other professionals in the planning phase of sewer system control design and effectively contribute to find novel control solution.

It was investigated if the established methodology used in classic control the-ory for process control design can be applied meaningfully to the sewer syst-tem. As the methodology takes its basis in a hierarchical decomposition of the control problem based on time-scale, it was also investigated if sewer sys-tem 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 sys-tem 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 setpoints 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 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.

**General information**

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**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.

**General information**

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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 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. The methodology employs a decomposition-based method so that the complexity of the problem 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 these reactive McCabe-Thiele and driving force method, 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 openloop 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.

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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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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 their 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).

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required reductions can be addressed through process synthesis-intensification-control, that is, the efficient use of raw materials (feedstock), the use of sustainable technologies and the design (and control) of processes that directly impact and improves sustainability/LCA factors. The unit operations concept, which has been sufficient until now, is one of the most used for performing process synthesis (and intensification) because it allows the association of tasks (functions) with the processing route to be followed. At the unit operations scale (Jaksland et al., 1995) and task scale (Sirola, 1996) alternatives are limited to existing (well-known) unit operations and therefore, may not be able to generate new integrations/combinations of intensified existing equipment.

However, to find innovative processes designs, extensions of the current concepts are necessary. Here, process synthesis-intensification using a phenomena based process synthesis method (Lutze et al., 2013) can play a major role because it provides the opportunity to perform the same tasks in a more sustainable way, new/novel unit operations can be generated (Lutze et al., 2013) and more sustainable processes can be designed (Babi et al., 2014).

An integrated, multi-stage, multi-scale, computer-aided framework has been developed in order to perform process synthesis-intensification-control. The framework operates at different scales, the unit operations scale, task scale and phenomena scale. In stage 1, process synthesis is performed (at the unit operations scale) using computer-aided flowsheet design (CAFD) (Tula et al., 2015), considering a superstructure of all possible alternatives based on known technologies, in order to generate a base case design. In stage 2, the base case design is decomposed into the smallest constituent units, that is, tasks then the involved phenomena. The base case design is analysed using economic and sustainability analyses in order to identify process limitations (hot-spots) that are translated into intensification design targets. In stage 3, an integrated task-phenomena-based synthesis-intensification method is embedded and applied (Babi et al., 2015) that consists of combining the phenomena to fulfil tasks, which are then translated into unit operations that constitute the (more sustainable) flowsheet alternatives which satisfy the intensification design targets. In this way, truly predictive and innovative solutions are generated much in the same way as atoms are combined to form molecules with desired properties (that is, analogous to computer-aided molecular design). The final stage involves validation and selection. Here detailed model-based calculations and/or experiments are performed to evaluate and compare the new solutions. In stage 4, design-control integration issues are validated/fine-tuned in order to generate the more sustainable controller structure. Note that in stages 1-3 design decisions are structured and made in such a way that the designed process(s) will also have the best opportunity for control (Mansouri et al., 2015).

In this presentation, the integrated process synthesis-intensification-control framework will be presented together with the corresponding databases, computer-aided models and tools needed to achieve sustainable synthesis-intensification. Different examples, related to synthesis, intensification and control will be presented for each stage of the framework.

**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.
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.

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 $V_f$ 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 experimental!) effort.
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.

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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 dependent on 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).
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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technische Universität Berlin, Politecnico di Milano
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 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.
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 as biorefineries [2]. The wide variety and complex nature of components in biorefineries poses 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.

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**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.

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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.

**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.

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**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.

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A Practical and Fast Method To Predict the Thermodynamic Preference of ω-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.

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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.
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) assessment of property model prediction 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.
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.

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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.
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 piggy 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.

General information
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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 monoxygenases. 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.

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.

Calibration and evaluation of predictive accuracy of a (micro)pollutant influent generator

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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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.
Challenges encountered calibrating N2O dynamics from mixed cultures

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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.

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**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.

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**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 limits, 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. WWTP layouts are currently developed based on expert and experience-based designs. However, as a result of the above-mentioned considerations, it is evident that making the most feasible decision with this experience-based approach will be increasingly difficult if not subjective. In this study, a systematic framework based on mathematical programming is proposed to handle the complex process synthesis problem by a superstructure optimization approach to generate a novel and optimal WWTP process selection for treatment of domestic wastewaters. 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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Computer-Aided Process Analysis for the Biocatalytic Production of an Antimicrobial Active Chemical

General information
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.

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.
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.

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Control Structure Design for an EBP2R Process Operated as a Sequencing Batch Reactor

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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.

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- Web of Science (2003): Indexed yes
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Densities of Pure Ionic Liquids and Mixtures: Modeling and Data Analysis

Our two-parameter corresponding states model for liquid densities and compressibilities has been extended to more pure ionic liquids and to their mixtures with one or two solvents. A total of 19 new group contributions (5 new cations and 14 new anions) have been obtained for predicting pressure effects over wide ranges of temperature and pressure. Comparisons of the technique with contemporary treatments based on equations of state show that it compares favorably with all other approaches.
Design of a process template for amine synthesis
A conceptual nitro reduction process template that should be generic such that it can handle a series of substrates with similar molecular functionality has been designed. The reduction process is based on a continuous plug-flow slurry reactor. The process template aims at speeding up the process development for new substrates by being easily adapted for a range of substrates as well as easily scaled by numbering-up. The potential saving in process development time could make it a particularly powerful experimental tool for early delivery campaigns in the pharmaceutical industry for the production of Kg amounts of material for clinical trials.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, CAPEC-PROCESS, Karlsruhe Institute of Technology KIT, AstraZeneca
Authors: Singh, R. (Intern), Godfrey, A. (External), Gregertsen, B. (External), Muller, F. (External), Vankayala, B. (External), Haas-Santo, K. (External), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
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Main Research Area: Technical/natural sciences
Generic process, Nitro reduction, Process template, Substrate adoption methodology, Fast process development, Flexible process, Pharmaceutical manufacturing process
Source: PublicationPreSubmission
Source-ID: 104282382
Publication: Research - peer-review › Report – Annual report year: 2014

Design of Separation Processes with Ionic Liquids
A systematic methodology for screening and designing of Ionic Liquid (IL)-based separation processes is proposed and demonstrated using several case studies of both aqueous and non-aqueous systems, for instance, ethanol + water, ethanol + hexane, benzene + hexane, and toluene + methycyclohexane. The best four ILs of each mixture are [mmim][dmp], [emim][bti], [emim][etso4] and [hmim][tcb], respectively. All of them were used as entrainers in the extractive distillation. A process simulation of each system was carried out and showed a lower both energy requirement and solvent usage as compared to conventional organic solvent process.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Chulalongkorn University
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Series: Computer - Aided Chemical Engineering
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 25th European Symposium on Computer Aided Process Engineering, Copenhagen, Denmark, 31/05/2015 - 31/05/2015
Development of an on-line state estimator for fed-batch filamentous fungal fermentations

Bioprocesses can be challenging to model due to complex and non-linear process dynamics [1]. In addition there is a lack of robust, on-line sensors for key parameters of interest in the field, such as substrate, product and biomass concentration [2]. These factors lead to limitations in the ability to monitor and control bioprocess systems. There is therefore an interest in state estimation, in order to model these key process states based on available on-line measurements [1].

This work discusses the application of a first principle model to pilot scale filamentous fungal fermentation systems operated at NovoZymes A/S. The model comprises of an online parameter estimation block, coupled to a physical model of the system. The parameter estimation block utilizes on-line off gas measurements and ammonia addition in order to model changing reaction rates in the system. Based on a global process stoichiometry, the current rates of product and biomass formation are identified [3]. This parameter estimate is then used as an input to a dynamic physical process model, which describes the mass transfer capabilities of the system based on the operating conditions, including stirrer speed, aeration rate and headspace pressure [4], [5].

This stoichiometric-based coupled process model is successfully applied on-line as a state estimator in order to predict the biomass and product concentration, from robust, available on-line measurements. Such state estimators will be valuable as part of control strategy development for on-line process control and optimization.

Development of Computer Aided Modelling Templates for Model Re-use in Chemical and Biochemical Process and Product Design: Important export of models

This paper focuses on the challenges in model development related to model reuse and compatibility and integration of different tools that are used in modelling. A link between two modelling tools, the computer-aided modelling framework of the ICAS system and the modelling environment, MOSAIC, has been established, in order to provide a wider range of modelling capabilities. Through this link, developed models can be exported/imported to/from other modelling-simulation software environments to allow model reusability in chemical and biochemical product and process design. The use of this link is illustrated through a case study.
Development of sustainable CO2 conversion processes for the methanol production

Utilization of CO2 feedstock through CO2 conversion for producing valuable chemicals as an alternative to sequestration of the captured CO2 is attracting increasing attention in recent studies. Indeed, the methanol production process via thermochemical CO2 conversion reactions is considered a prime candidate for commercialization. The aim of this study is to examine two different options for a sustainable methanol plant employing the combined reforming and CO2 hydrogenation reactions, respectively. In addition, process improvement strategies for the implementation of the developed processes are also considered. The two methanol plants are developed using Aspen Plus®, the commercial process simulator. The net CO2 flows and methanol production costs are evaluated using ECON® and compared with those of the conventional methanol plant, which uses two-stage reforming. It is verified that the combined reforming process has to be integrated with the existing conventional methanol plant to obtain a reduced CO2 emission as well as lowered production costs. On the other hand, the CO2 hydrogenation based methanol plant could achieve a reduction of net CO2 emission at a reasonable production cost only with utilization of renewable energy resources (hydroelectric power and biomass) for the H2 feedstock.

Dynamic Modeling and Validation of a Biomass Hydrothermal Pretreatment Process - A Demonstration Scale Study

Hydrothermal pretreatment of lignocellulosic biomass is a cost effective technology for second generation biorefineries. The process occurs in large horizontal and pressurized thermal reactors where the biomatrix is opened under the action of steam pressure and temperature to expose cellulose for the enzymatic hydrolysis process. Several by-products are also formed, which disturb and act as inhibitors downstream. The objective of this study is to formulate and validate a large scale hydrothermal pretreatment dynamic model based on mass and energy balances, together with a complex conversion mechanism and kinetics. The study includes a comprehensive sensitivity and uncertainty analysis, with parameter estimation from real-data in the 178-185° range. To highlight the application utility of the model, a state estimator for biomass composition is developed. The predictions capture well the dynamic trends of the process, outlining the value of the model for simulation, control design, and optimization for full-scale applications.
Dynamic Modeling of Pectin Extraction for Monitoring and Optimization

Pectin is used as an additive in many food and pharmaceutical products to modify the rheological properties of the product [1]. Commercial pectin extraction is a batch operation with several tanks that can feed continuously the downstream processing. The variability of the raw material is a continuous input of uncontrolled disturbances to the process. Consequently, the process conditions should be constantly adjusted in order to obtain a high pectin yield and good product quality. The pectin quality can be characterized by the degree of esterification (%DE) [2]. Measurements of %DE can only be carried out after precipitation, which occurs several hours from the start of extraction. As a consequence, some batches are processed under non-optimal conditions reducing pectin yield and quality.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CP Kelco ApS
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Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

Dynamic Modeling, Optimization, and Advanced Control for Large Scale Biorefineries

Second generation biorefineries transform agricultural wastes into biochemicals with higher added value, e.g. bioethanol, which is thought to become a primary component in liquid fuels [1]. Extensive endeavors have been conducted to make the production process feasible on a large scale, and recently several commercial size biorefineries became operational: Beta Renewables (Italy, 2014), Abengoa Bioenergy (USA, 2014), POET-DSM (USA, 2014), GranBio (Brazil, 2014) [2], while others are under construction, e.g. the Måbjerg Energy Consortium in Denmark. This thesis presents the findings of a 3 years PhD project that was run by Technical University of Denmark (DTU) in collaboration with the largest Danish energy company DONG Energy A/S between 2012 and 2015. The company owns a demonstration scale second generation biorefinery in Kalundborg, Denmark, also known as the Inbicon demonstration plant [3]. The goal of the project is to utilize realtime data extracted from the large scale facility to formulate and validate first principle dynamic models of the plant. These models are then further exploited to derive model-based tools for process optimization, advanced control and realtime monitoring. The Inbicon biorefinery converts wheat straw into bioethanol utilizing steam, enzymes, and genetically modified yeast. The biomass is first pretreated in a steam pressurized and continuous thermal reactor where lignin is relocated, and hemicellulose partially hydrolyzed such that cellulose becomes more accessible to enzymes. The biorefinery is integrated with a nearby power plant following the Integrated Biomass Utilization System (IBUS) principle for reducing steam costs [4]. During the pretreatment, by-products are also created such as organic acids, furfural, and pseudo-lignin, which act as inhibitors in downstream processes. The pretreated fibers consist of cellulose and xylan, which are then liquefied in the enzymatic hydrolysis process with the help of enzymes. High glucose and xylose yields are thus obtained for co-fermentation. Ethanol is recovered in distillation columns followed by molecular sieves for achieving a high concentration ethanol. Lignin is separated in the first column and recovered as bio-pellets in an evaporation unit. The bio-pellets are then burnt in the nearby power plant for steam generation. The first part of this research presents a large scale dynamic model of the plant, separated in modules for pretreatment, enzymatic hydrolysis, and fermentation. The pretreatment and enzymatic hydrolysis models have been validated and analyzed in this study together with a comprehensive sensitivity and uncertainty analysis [5, 6]. The models embed mass and energy balances with a complex conversion route. Computational fluid dynamics is used to model transport phenomena in large reactors capturing tank
profiles, and delays due to plug flows. This work publishes for the first time demonstration scale real data for validation showing that the model library is suitable for optimization, control and monitoring purposes. As an application, the pretreatment dynamic model is used to construct a realtime observer that acts both as a measurement filter, and soft sensor for biomass components that are not measured, e.g. pretreatment inhibitors [5]. The next part of this study deals with building a plantwide model-based optimization layer, which searches for optimal values regarding the pretreatment temperature, enzyme dosage in liquefaction, and yeast seed in fermentation such that profit is maximized [7]. When biomass is pretreated, by-products are also created that affect the downstream processes acting as inhibitors in enzymatic hydrolysis and fermentation. Therefore, the biorefinery is treated in an integrated manner capturing the trade-offs between the conversion steps. Sensitivity and uncertainty analysis is also performed in order to identify the modeling bottlenecks and which feedstock components need to be determined for an accurate prediction. This analysis is achieved with Monte Carlo simulations and Latin Hypercube Sampling (LHS) on feedstock composition and kinetic parameters following the methodology from [5, 6, 8, 9]. In the last part of this work, two applications of the L1 adaptive output feedback controller [10] are developed: one for biomass pretreatment temperature [11] and another one for pH in enzymatic hydrolysis [12]. Biomass conversion is highly sensitive to these process parameters, which exhibit nonlinear behavior and can change nominal values. The adaptive controllers are found to perform better across multiple operational points without the need of retuning.

General information
State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, DONG Energy A/S
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Number of pages: 244
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Publisher: Technical University of Denmark, Department of Electrical Engineering
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Projects:
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Publication: Research › Ph.D. thesis – Annual report year: 2016

Dynamic Modelling and Identification of Precipitation Reactions in Full-Scale WWTP
Current process models used across the wastewater industry have inherent limitations due to limited description of physicochemical processes such as precipitation. As part of the overall effort towards more general and robust physicochemical models applicable to the broad range of problems, this paper evaluates plant-wide modelling of precipitation reactions using a generic approach integrated within activated sludge and anaerobic models. Preliminary results of anaerobic digester sludge in batch system suggest that the model is able to simulate the dynamics of precipitation reactions. Kinetic rate coefficients, identified by mathematical optimization, were 4.65(±0.74) hrs- and 2.98(±0.48) hrs- for struvite and amorphous calcium phosphate (ACP), respectively. The joint parameter confidence regions found were highly nonlinear and asymmetric, indicating that the model was more tolerant to a fast kinetic coefficient. Nonlinearity of the confidence regions also indicates that nonlinear and iterative techniques for parameter identification are required in estimating real parameter uncertainty. Additional experimental results and model analysis in full-scale WWTP will be presented in the full paper.

General information
State: Published
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Number of pages: 4
Publication date: 2015
Event: Abstract from 9th IWA Symposium on Systems Analysis and Integrated Assessment (Watermatex 2015), Gold Coast, Queensland, Australia.
Main Research Area: Technical/natural sciences
Physico-chemical modelling, Precipitation kinetics, Parameter estimation
Electronic versions: kazadi_watermatex_2015.pdf
Economic Considerations for Selecting an Amine Donor in Biocatalytic Transamination

The industrial implementation of biocatalysis for production of pharma and fine chemicals has grown substantially over recent years. An upcoming application is that of chiral synthesis of optically pure amines, a technology known for many years but that is now seeing a renewed and wider interest in industry. The technology has been demonstrated in a few selected cases, but widespread implementation and for a broader range of target molecules requires a deeper understanding of the underlying thermodynamic as well as economic constraints for the different choices that can be made in designing the process, in particular the choice of amine donor. This paper discusses these constraints and demonstrates, through simple thermodynamic and economic models, the process targets that need to be set and achieved for a process dependent on allowed process costs and quality targets.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, DSM Innovative Synthesis, CLEcta GmbH, Sigma-Aldrich Chemie GmbH
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Pages: 652-660
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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
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
Effects of influent fractionation, kinetics, stoichiometry and mass transfer on CH₄, H₂ and CO₂ production for (plant-wide) modeling of anaerobic digesters

This paper examines the importance of influent fractionation, kinetic, stoichiometric and mass transfer parameter uncertainties when modeling biogas production in wastewater treatment plants. The anaerobic digestion model no. 1 implemented in the plant-wide context provided by the benchmark simulation model no. 2 is used to quantify the generation of CH₄, H₂ and CO₂. A comprehensive global sensitivity analysis based on (i) standardized regression coefficients (SRC) and (ii) Morris' screening's (MS's) elementary effects reveals the set of parameters that influence the biogas production uncertainty the most. This analysis is repeated for (i) different temperature regimes and (ii) different solids retention times (SRTs) in the anaerobic digester. Results show that both SRC and MS are good measures of sensitivity unless the anaerobic digester is operating at low SRT and mesophilic conditions. In the latter situation, and due to the intrinsic nonlinearities of the system, SRC fails in decomposing the variance of the model predictions (R² < 0.7) making MS a more reliable method. At high SRT, influent fractionations are the most influential parameters for predictions of CH₄ and CO₂ emissions. Nevertheless, when the anaerobic digester volume is decreased (for the same load), the role of acetate degraders gains more importance under mesophilic conditions, while lipids and fatty acid metabolism is more influential under thermophilic conditions. The paper ends with a critical discussion of the results and their implications during model calibration and validation exercises.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University
Authors: Solon, K. (Ekstern), Flores Alsina, X. (Intern), Gernaey, K. (Intern), Jeppsson, U. (Ekstern)
Pages: 870-877
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Main Research Area: Technical/natural sciences

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Journal: Water Science and Technology
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Web of Science (2017): Indexed yes
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
Effects of ionic strength and ion pairing on (plant-wide) modelling of anaerobic digestion

Plant-wide models of wastewater treatment (such as the Benchmark Simulation Model No. 2 or BSM2) are gaining popularity for use in holistic virtual studies of treatment plant control and operations. The objective of this study is to show the influence of ionic strength (as activity corrections) and ion pairing on modelling of anaerobic digestion processes in such plant-wide models of wastewater treatment. Using the BSM2 as a case study with a number of model variants and cationic load scenarios, this paper presents the effects of an improved physico-chemical description on model predictions
and overall plant performance indicators, namely effluent quality index (EQI) and operational cost index (OCI). The acid-base equilibria implemented in the Anaerobic Digestion Model No. 1 (ADM1) are modified to account for non-ideal aqueous-phase chemistry. The model corrects for ionic strength via the Davies approach to consider chemical activities instead of molar concentrations. A speciation sub-routine based on a multi-dimensional Newton-Raphson (NR) iteration method is developed to address algebraic interdependencies. The model also includes ion pairs that play an important role in wastewater treatment. The paper describes: 1) how the anaerobic digester performance is affected by physico-chemical corrections; 2) the effect on pH and the anaerobic digestion products (CO2, CH4 and H2); and, 3) how these variations are propagated from the sludge treatment to the water line. Results at high ionic strength demonstrate that corrections to account for non-ideal conditions lead to significant differences in predicted process performance (up to 18% for effluent quality and 7% for operational cost) but that for pH prediction, activity corrections are more important than ion pairing effects. Both are likely to be required when precipitation is to be modelled.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University, University of Queensland, Ghent University
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Main Research Area: Technical/natural sciences

**Publication Information**

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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
Estimation and Uncertainty Analysis of Flammability Properties for Computer-aided molecular design of working fluids for thermodynamic cycles

Computer Aided Molecular Design (CAMD) is an important tool to generate, test and evaluate promising chemical products. CAMD can be used in thermodynamic cycle for the design of pure component or mixture working fluids in order to improve the heat transfer capacity of the system. The safety assessment of novel working fluids relies on accurate property data. Flammability data like the lower and upper flammability limit (LFL and UFL) play an important role in quantifying the risk of fire and explosion. For novel working fluid candidates experimental values are not available for the safety analysis. In this case property prediction models like group contribution (GC) models can estimate flammability data. The estimation needs to be accurate, reliable and as less time consuming as possible [1]. However, GC property prediction methods frequently lack rigorous uncertainty analysis. Hence, there is no information about the reliability of the data. Furthermore, the global optimality of the GC parameters estimation is often not ensured.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Frutiger, J. (Intern), Abildskov, J. (Intern), Sin, G. (Intern)
Number of pages: 2
Publication date: 2015
Event: Abstract from CAPE Forum 2015, Paderborn, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
Jerome_Frutiger_Abstract_CAPE15.docx
Source: PublicationPreSubmission
Source-ID: 110149021
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Estimation and Uncertainty Analysis of Flammability Properties of Chemicals using Group- Contribution Property Models

Process safety studies and assessments rely on accurate property data. Flammability data like the lower and upper flammability limit (LFL and UFL) play an important role in quantifying the risk of fire and explosion. If experimental values are not available for the safety analysis due to cost or time constraints, property prediction models like group contribution (GC) models can estimate flammability data. The estimation needs to be accurate, reliable and as less time consuming as possible. However, GC property prediction methods frequently lack rigorous uncertainty analysis. Hence, there is no information about the reliability of the data. Furthermore, the global optimality of the GC parameters estimation is often not
ensured.

In this research project, flammability-related property data, like LFL and UFL, are estimated using the Marrero and Gani group contribution method (MG method). In addition to the parameter estimation, an uncertainty analysis of the estimated data and a comparison to other methods is performed. A thorough uncertainty analysis provides information about the prediction error, which is important for the use of the data in process safety studies and assessments.

The method considers the group contribution in three levels: The contributions from a specific functional group (1st order parameters), from polyfunctional (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.

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.

In this study, the MG-GC-factors are estimated using a systematic data and model evaluation methodology in the following way:

1) Data. Experimental flammability data is used from AIChE DIPPR 801 Database.
2) Initialization and sequential parameter estimation. An approximation using linear algebra provides the first guess. Then the 1st, 2nd and 3rd order parameter estimations are performed separately.
3) Simultaneous parameter estimation. The result of the sequential estimation serves then as initial guess for the simultaneous parameter estimation algorithm. Different minimization/search algorithms ensure global optimality.
4) Uncertainty. A rigorous uncertainty analysis that includes asymptotic approximation of covariance matrix for parameter estimators is performed in order to provide information of the model prediction quality (95% confidence interval).

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Frutiger, J. (Intern), Abildskov, J. (Intern), Sin, G. (Intern)
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Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 103338139
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Evaluation of an in-line particle imaging tool for monitoring twin-screw granulation performance

Twin-screw granulation is an emerging continuous wet granulation technique in the pharmaceutical industry due to several advantages over batch granulation. However, for the implementation of a fully continuous line in an industrial environment, in-process measurement tools are required to monitor critical process parameters and (intermediate) product quality attributes, and trigger control actions based on such measurements. This study aimed at evaluating the feasibility of implementing an in-line particle imaging technique (Eyecon™) after continuous twin-screw granulation and before the drying system. Off-line sieving was used as reference particle size analysis method. A twin-screw granulator which is part of the Consigma system was used to granulate a placebo formulation composed of lactose and polyvinylpyrrolidone (PVP; 97.5:2.5% w/w). PVP was dissolved in water, which was used as granulation liquid at liquid-to-solid ratios ranging between 8 and 9%. The performance of the in-line measurement method at heterogeneous process conditions was tested by changing the liquid to solid ratio (8–9%), the material throughput (10–25 kg/h) and the screw configuration (16 and 26 kneading discs). The volumetric size distribution obtained from the in-line measurements of the granules leaving the twin-screw granulator using the Eyecon™ camera was compared with the off-line measurements obtained by sieving of the granule samples collected before and after the drying unit operation. For the intermediate size range (diameter 250–1000 μm), the Eyecon™ measurements showed to be promising as they were in agreement with off-line measurement results obtained before the drying unit. However, the image analysis algorithm and data post-processing of the Eyecon™ images for the fines and oversized ranges require modification for improvement in measurement results. In conclusion, the Eyecon™ provides very good in-line images despite adverse moving flow of granules. However, proper analysis of these images is crucial before application as standard in-line particle size monitoring tool and application for control purposes can be realized.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Ghent University
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Pages: 80-87
Publication date: 2015
Main Research Area: Technical/natural sciences
Experimental and in-silico investigation of population heterogeneity in continuous Sachharomyces cerevisiae scale-down fermentation in a novel two-compartment setup.

BACKGROUND: In large-scale bioreactors, microbes often encounter fluctuating conditions of nutrient and oxygen supply, resulting in different microbial behavior at the different scales. The underlying reason is spatial heterogeneity, caused by limited mixing capabilities at production scale. Consequently, scale-up of processes is challenging and there is a need for laboratory-scale reactor setups that can mimic large-scale conditions to enhance the understanding of how fluctuating environmental conditions affect microbial physiology.

RESULTS: A two-compartment, scale-down setup, consisting of two interconnected stirred tank reactors was used in combination with mathematical modeling, to mimic large-scale continuous cultivations. One reactor represents the feeding zone with high glucose concentration and low oxygen, whereas the other one represents the remaining reactor volume. An earlier developed population balance model coupled to an unstructured model was used to describe the development of bulk concentrations and cell size distributions at varying dilution rate, glucose feed concentration as well as recirculation times between the two compartments. The concentration profiles of biomass and glucose were successfully validated experimentally. Single cell properties of two fluorescent reporter strains that were applied for deeper investigation of cell robustness characteristics and ethanol growth distributions were quantified compartment-wise revealing differences in cell population distributions related to environmental conditions and also compared with the one-compartment, conventional chemostat.

CONCLUSION: Results underline the utility for the proposed combined approach as well as the use of continuous scale-down reactors for process investigations as insights concerning single-cell characteristics of the process are revealed, which are normally hidden.

General information
State: Published
Organisations: Metabolic Signaling and Regulation, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CHEC Research Centre
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Pages: 324-340
Publication date: 2015
Main Research Area: Technical/natural sciences

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Volume: 90
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 2.94 SJR 0.843 SNIP 1.111
Web of Science (2016): Indexed yes
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
In this work the Benchmark Simulation Model No.2 is extended with processes for nitrous oxide production and for side-stream partial nitritation/Anammox (PN/A) treatment. For these extensions the Activated Sludge Model for Greenhouse gases No.1 was used to describe the main waterline, whereas the Complete Autotrophic Nitrogen Removal (CANR) model was used to describe the side-stream (PN/A) treatment. Comprehensive simulations were performed to assess the extended model. Steady-state simulation results revealed the following: (i) the implementation of a continuous CANR side-stream reactor has increased the total nitrogen removal by 10%; (ii) reduced the aeration demand by 16% compared to the base case, and (iii) the activity of ammonia-oxidizing bacteria is most influencing nitrous oxide emissions. The extended model provides a simulation platform to generate, test and compare novel control strategies to improve operation performance and to meet the new plant performance criteria such as minimization of greenhouse gas (in particular of nitrous oxide) emissions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Boiocchi, R. (Intern), Sin, G. (Intern), Gernaey, K. V. (Intern)
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Formulation and Design of a CO2 Utilization Network Detailed Through a Conceptual Example

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 sustainability and feasibility of linking carbon capture and CO2 conversion is studied in detail in a case study. CCS is still under development and CO2 utilization is showing great promise as an additional method of combatting CO2 emissions [2]. 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. The network also links carbon capture to ensure the sustainability. 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. 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, the network is analyzed in the conceptual example of methanol synthesis via CO2 hydrogenation. 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.

General information
State: Published
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Formulation of a Network and the Study of Reaction Paths for the Sustainable Reduction of CO2 Emissions
Various organizations, especially the Intergovernmental Panel on Climate Change, have stated that global warming is an ever-increasing threat to the environment and poses a problem if not addressed. Therefore, efforts are being made to find methods of reducing contributors to global warming, primarily greenhouse gas emissions. Of these, carbon dioxide (CO2) is the largest source and, hence, the reduction of the amount emitted is primary focus of developments [1]. A new and promising process that reduces the emissions is the conversion of CO2 into useful products, such as methanol and dimethyl carbonate (DMC) [2].

In this work, through a computer-aided framework for process network synthesis-design, a network of conversion processes that all use emitted CO2 is investigated. CO2 is emitted into the environment from various sources: power generation, industrial processes, transportation and commercial processes. Within these there are high-purity emissions and low-purity emissions. Rather than sending these to the atmosphere, it is possible to collect them and use them for other purposes. Targeting some of the largest contributors: power generation, manufacturing, chemical industry, it is possible to determine the amounts available. Once the CO2-sources are known, it is possible to determine how to utilize these through process network optimization.

In addition to the source information, reaction details are vital. Understanding the conversions that are thermodynamically
feasible, process co-reactants, catalysts necessary, operating conditions and reactions, is the next step. The products that are formed fall into categories: fuels, bulk chemicals and specialty chemicals. While fuels, such as methanol (MeOH), have the largest market, this network will include a variety of thermodynamically feasible conversion paths [3]. From reviews of work previously done, there are ranges of possible products that are formed directly from CO2 and another co-reactant. Methanol, dimethyl ether, dimethyl carbonate and ethylene carbonate are just some of the products that can be formed.

With the information of sources and reactions, a tree of reaction paths is formed and investigated. This forms a superstructure of CO2 utilization to a variety of products. Each of the paths in the network involves CO2 and a co-reactant, such as hydrogen, which may also be captured from process purge streams. The process network evolves as some of the reactions involve products from other reactions as a reactant. Combining the possible products that can be formed and the reactants that are required yields a network of products that can be created using only the CO2 emissions and not adding any CO2 emissions through the reactions.

Studies and detailed simulations have been performed on CO2 conversion to methanol, synthesis gas processes, dimethyl carbonate production, and other processes. The detailed simulations are performed on the paths that are selected based on basic calculations on each path. Then, those paths that are targeted from base calculations are further simulated for detailed information. From these detailed simulations, results are provided, enhancing the superstructure for an improved analysis. In addition, the aim is to create sustainable alternatives for the production of these products with an overall reduction of CO2, both in the material and energy streams. With the use of computer-aided tools, this network, and the information contained within it, is generated. The detailed simulations, of CO2 conversion to methanol, synthesis gas production and DMC manufacture, provide in-depth knowledge of the various paths that are most promising. The economic feasibility and sustainability are assessed to identify the final, more sustainable network. Overall, the target is the formation of a network that reduces emissions by forming desirable chemical products without emitting noticeable amounts of CO2 and other greenhouse gases, and creating more energy efficient processes.

General Information
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From Fed-batch to Continuous Enzymatic Biodiesel Production
In this this paper, we use mechanistic modelling to guide the development of acontinuous enzymatic process that is performed as a fed-batch operation. In this work we use the enzymatic biodiesel process as a case study. A mechanistic model developed in our previous work was used to determine the reactor operating conditions for a desired conversion. However, in using a detailed mechanistic model, given the large number of parameters and few experimental data points, the parameters were found not identifiable. The model is then only applicable within the limited operating range for which the model was validated. We hypothesize that fitting this model to fed-batch and continuous stirred tank reactor (CSTR) data together will enable us to use the model for determination of residence times to reach a specified conversion in a CSTR. With this approach, the model fits the experimental data for the five measured components (triglycerides, diglycerides, monoglycerides, free fatty acid and fatty acid methyl esters(biodiesel)) much better than using fed-batch data alone given the smaller residuals. We also observe a reduction in the correlation between the parameters. The model was then used to predict that 5 reactors are required (with a combined residence time of 30 hours) to reach a final biodiesel concentration within 2 % of the 95.6 mass % achieved in a fed-batch operation, for 24 hours.

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Pages: 1337-1342
Publication date: 2015
Fungal Morphology in Industrial Enzyme Production - Modelling and Monitoring

Filamentous fungi are widely used in the biotechnology industry for the production of industrial enzymes. Thus, considerable work has been done with the purpose of characterizing these processes. The ultimate goal of these efforts is to be able to control and predict fermentation performance on the basis of "standardized" measurements in terms of morphology, rheology, viscosity, mass transfer and productivity. However, because the variables are connected or dependent on each other, this task is not trivial. The aim of this review article is to gather available information in order to explain the interconnectivity between the different variables in submerged fermentations. An additional factor which makes the characterization of a fermentation broth even more challenging is that the data obtained are also dependent on the way they have been collected-meaning which technologies or probes have been used, and on the way the data is interpreted-i.e. which models were applied. The main filamentous fungi used in industrial fermentation are introduced, ranging from Trichoderma reesei to Aspergillus species. Due to the fact that secondary metabolites, like antibiotics, are not to be considered bulk products, organisms like e.g. Penicillium chrysogenum are just briefly touched upon for the description of some characterization techniques. The potential for development of different morphological phenotypes is discussed as well, also in view of what this could mean to productivity and-equally important-the collection of the data. An overview of the state of the art techniques for morphology characterization is provided, discussing methods that finally can be employed as the computational power has grown sufficiently in the recent years. Image analysis (IA) clearly benefits most but it also means that methods like near infrared measurement (NIR), capacitance and on-line viscosity now provide potential alternatives as powerful tools for characterizing morphology. These measuring techniques, and to some extent their combination, allow obtaining the data necessary for supporting the creation of mathematical models describing the fermentation process. An important part of this article will indeed focus on describing the different models, and on discussing their importance to fermentations of filamentous fungi in general. The main conclusion is that it has not yet been attempted to develop an overarching model that spans across strains and scales, as most studies indeed conclude that their respective results might be strain specific and not necessarily valid across scales.
Generation of synthetic influent data for performing (micro) pollutant wastewater treatment modelling studies

The use of Activated Sludge Models (ASM) (Henze et al., 2000) is constantly growing and both industry and academia are increasingly applying these tools when performing wastewater treatment plant (WWTP) engineering studies. Besides describing the behaviour of traditional pollutants such as organic carbon (C), nitrogen (N) and phosphorus (P), ASM models have been successfully upgraded to predict the fate of different types of micro-pollutants (Benedetti et al., 2013). Indeed, the potential adverse effects of micro-pollutants in aquatic environments have been an object of intensive research during the last years (e.g. Ferrari et al., 2003). However, due to the time and the high cost of measuring campaigns, many simulation studies of full-scale Wastewater Treatment Plants (WWTPs) suffer from a lack of sufficiently long and detailed time series representing realistic wastewater influent dynamics (Gernaey et al., 2011). This is an important point since realistic data representing the influent wastewater dynamics are crucial to accomplish any WWTP modelling project (Rieger et al., 2012). For this reason, model-based influent generators/synthetic data are an alternative that has recently gained considerable interest (Flores-Alsina et al., 2014, Martin and Vanrolleghem 2014).

The objective of this paper is to show the usefulness of model based influent generators to reproduce (micro) pollutant influent characteristics when performing WWTP modelling studies. Using a 30000 PE WWTP as a case base, three different types of pharmaceuticals (antibiotic, anti-inflammatory, model stabilizer) are the selected micro-pollutant to run the study. In addition, the paper is complemented describing the influent variation of flow-rate (Q), traditional pollutants (COD, N, P) and temperature (T). Two different data sets (short/long term) are used to calibrate the different model blocks comprising the influent generator. Preliminary simulation results show that the generated synthetic data follows the same pollutant/micro-pollutant dynamics. In addition, uncertainty in the assumed loads/natural stochasticity is assessed using the Monte Carlo simulation technique. The paper will be complemented with a scenario analysis demonstrating how additional influent characteristics (following the same catchment) principles could be generated without the need to run (expensive) additional experimental campaigns.

General information
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Authors: Snip, L. J. P. (Intern), Aymerich, I. (Ekstern), Flores-Alsina, X. (Intern), Jeppsson, U. (Ekstern), Plósz, B. G. (Intern), Corominas, L. (Ekstern), Gernaey, K. V. (Intern)
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Publications: Research - peer-review › Article in proceedings – Annual report year: 2015

Generic Mathematical Programming Formulation and Solution for Computer-Aided Molecular Design

This short communication presents a generic mathematical programming formulation for Computer-Aided Molecular Design (CAMD). A given CAMD problem, based on target properties, is formulated as a Mixed Integer Linear/Non-Linear Program (MILP/MINLP). The mathematical programming model presented here, which is formulated as an MILP/MINLP problem, considers first-order and second-order molecular groups for molecular structure representation and property estimation. It is shown that various CAMD problems can be formulated and solved through this model.

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BFI (2016): BFI-level 2
Scopus rating (2016): SJR 1.122 SNIP 1.724 CiteScore 3.04
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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 1.293 SNIP 2.127
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
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.073 SNIP 1.113
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Electronic versions:
1_s2.0_S0098135415001234_main_2_.pdf. Embargo ended: 01/05/2017
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10.1016/j.compchemeng.2015.04.022
Guidelines for development and implementation of biocatalytic P450 processes

Biocatalytic reactions performed by cytochrome P450 monooxygenases are interesting in pharmaceutical research since they are involved in human drug metabolism. Furthermore, they are potentially interesting as biocatalysts for synthetic chemistry because of the exquisite selectivity of the chemistry they undertake. For example, selective hydroxylation can be undertaken on a highly functionalized molecule without the need for functional group protection. Recent progress in the discovery of novel P450s as well as protein engineering of these enzymes strongly encourages further development of their application, including use in synthetic processes. The biological characteristics of P450s (e.g., cofactor dependence) motivate the use of whole-cell systems for synthetic processes, and those processes implemented in industry are so far dominated by growing cells and native host systems. However, for an economically feasible process, the expression of P450 systems in a heterologous host with sufficient biocatalyst yield (g/g cdw) for non-growing systems or space-time yield (g/L/h) for growing systems remains a major challenge. This review summarizes the opportunities to improve P450 whole-cell processes and strategies in order to apply and implement them in industrial processes, both from a biological and process perspective. Indeed, a combined approach of host selection and cell engineering, integrated with process engineering, is suggested as the most effective route to implementation.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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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
Hydrodynamic Characterization of Substrate Gradients in a Pilot Scale Fermenter Using CFD and Spatially Distributed Sensors

The prediction and understanding of mixing and oxygen mass transfer in fermenters and bioreactors is useful for bioprocess improvement as these dynamics govern production rates of the biotransformation. In particular heterogeneities occurring under process conditions is of interest as such gradients present challenges for process development and scale up [1]. Heterogeneities in substrate concentration have been identified in large scale fermenters [2] and reliable tools to identify and quantify these phenomena are required. This work utilizes the degradation of hydrogen peroxide to oxygen by catalase to illustrate and validate how substrate is distributed throughout the vessel by combining CFD and experimental data collected with spatially distributed sensors.

General information
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Immobilisation of ω-transaminase for industrial application: Screening and characterisation of commercial ready to use enzyme carriers

Despite of the advantages that enzyme immobilisation can bring to industrial biocatalysis, its utilisation is still limited to a small number of enzymes and processes. Transaminase catalysed processes are a good example where immobilisation can be of major importance and even decisive for economic feasibility. This work presents results obtained for screening of enzyme carriers for immobilisation of ω-transaminase for industrial application. A total of 6 commercial enzyme carriers (polymeric resins) were screened and two suitable enzyme carriers were selected for immobilisation of both (S)- and (R)-selective ω-transaminases. These carriers allowed the re-use of the immobilised enzyme for 8 cycles of 24 h each, under relevant process conditions, corresponding to approximately 250 h of operation, with more than 50% of the initial activity retained. Likewise the stability towards higher temperatures and possibility to store the biocatalyst for more than 70 days (at room temperature) were obtained as result of the immobilisation on the selected supports.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, C-LEcta GmbH, DSM Innovative Synthesis
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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
Scopus rating (2009): SJR 0.898 SNIP 1.136
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.975 SNIP 1.021
Web of Science (2008): Indexed yes
Industrial wastewater treatment network based on recycling and rerouting strategies for retrofit design schemes

The advent of complex industrial water/wastewater management problems points to a need for effective systematic design for a sustainable solution. The objective of this work is to extend the research in the area of systematic design of water/wastewater management by further developing and extending a generic model-based synthesis and design framework for retrofit wastewater treatment networks (WWTN) of an existing industrial process. The developed approach is suitable for grassroots and retrofit systems and adaptable to a wide range of wastewater treatment problems. A sequential solution procedure is employed to solve a network superstructure-based optimization problem formulated as Mixed Integer Linear and/or Non-Linear Programming (MILP/MINLP). Data from a petroleum refinery effluent treatment plant together with special design constraints are employed to formulate different design schemes based on recycling and rerouting strategies focusing on completely splitting system and zero liquid discharge (ZLD) opportunity. The base case design of the existing process has been verified against the refinery data, while the grassroots and the retrofit options are generated and compared with the existing process. The network design solutions obtained with effectively computational time from the case study shows an improvement in the reduction of a total annualized cost (TAC) and wastewater discharge rate (WWDR) as a result of water recycling and rerouting options. Pareto plot (trade-off solution graph) for the analysis of such optimal solutions has been applied to implicitly verify the optimality of the solution based on all possible scenarios. Superior retrofit alternatives have been identified based on their performance including cost and environmental impacts and can be used as efficient design guidelines for the future development of the existing wastewater treatment process.

General information
State: Published
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Scopus rating (2016): CiteScore 5.83 SJR 1.615 SNIP 2.382
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Integrated Design and Control of Reactive and Non-Reactive Distillation 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 (Huusom, 2015). 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) (Hamid et al., 2010) as well as complex chemical processes; for example, intensified processes such as reactive distillation (Mansouri et al., 2015). 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 (Sharifzadeh, 2013).

In this work, integrated design and control of non-reactive distillation, ternary compound reactive distillation and multi-component reactive distillation processes is considered systematically 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 any kind of imposed disturbance under normal operating conditions. First, to design non-reactive binary distillation columns, a set of conventional and simple design methods such as McCabe-Thiele and driving force approach (Bek-Pedersen and Gani, 2004) are selected. Next, these design methods are extended using element concept to also include ternary as well as multicomponent reactive distillation processes. The element concept (Pérez Cisneros et al., 1997) is used to translate a ternary system of compounds (A + B ↔ C) to a binary system of element (WA and WB). In the case of multicomponent reactive distillation processes the equivalent element concept is used to translate a multicomponent (multi-element) system (Jantharasuk et al., 2011) of compounds (A + B ↔ C + D(inert)) to a binary system of key elements (elements WHK and WLK). For an energy-efficient design, non-reactive driving force (for binary non-reactive distillation), reactive driving force (for ternary compound reactive distillation) 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 (except for binary non-reactive distillation column). ICAS-PDS is used to compute the reactive vapor-liquid equilibrium data set by consecutive calculation of reactive bubble points. It has been shown previously that designing a reactive distillation column at the maximum driving force will result in the minimum energy consumption (Bek-Pedersen and Gani, 2004). Note, that the same principles that apply to a binary non-reactive compound system are valid also for a binary-element or a binary-key-element system. Therefore, it is advantageous to employ the element based method for multicomponent reaction-separation systems.

The operation of the non-reactive distillation column, ternary reactive distillation column (binary-element) and multicomponent reactive distillation column (binary-key-element) is investigated at the highest driving force and other candidate points. It is shown analytically and through rigorous dynamic process simulation (using ICAS process simulation software and Aspen Plus) for all three cases that the sensitivity of the system to the disturbances in the feed at the highest driving force is less than any other candidate point. By application of this approach, it is shown that designing the non-reactive and reactive distillation processes at the maximum driving force results in an optimal design in terms of controllability and operability as well as an optimal/near optimal design from an energy point of view. 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.

**General information**
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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), Gani, R. (Intern)
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**Integrated Process Design and Control of Reactive Distillation Processes**
In this work, integrated design and control of reactive distillation processes is presented. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used, such as reactive McCabe-Thiele method and driving force approach. The methods are based on the element concept, which is used to translate a system of compounds into elements. The operation of the reactive distillation column at the highest driving force and other candidate points is analyzed through analytical solution as well as rigorous open-loop and closed-loop simulations. By application of this approach, it is shown that designing the reactive distillation process at the maximum driving force results in an optimal design in terms of controllability and operability. 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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana
Integrated Process Design and Control of Reactive Distillation Processes

In this work, integrated process design and control of reactive distillation processes is presented. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used, such as reactive McCabe-Thiele method and driving force approach. The methods are based on the element concept, which is used to translate a system of compounds into elements. The operation of the reactive distillation column at the highest driving force and other candidate points is analyzed through analytical solution as well as rigorous open-loop and closed-loop simulations. By application of this approach, it is shown that designing the reactive distillation process at the maximum driving force results in an optimal design in terms of controllability and operability. 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.

Investigation of a Gas-Solid Separation Process for Cement Raw Meal

The gas/solid heat exchanger (2D-HX), developed to replace the cyclone preheaters in cement plants is presented. This design aims at reducing construction height and operation costs. The separation process in the 2D-HX is experimentally investigated, and the results show that separation efficiencies up to 90% can be achieved in the gravitationally driven process. Based on the data, a model of the separation process is developed, utilizing relations from pneumatic transport and cyclone theory. The model fit is acceptable, especially in the area of interest. Based on experimental data, further development of the technology is encouraged.
Kinetic modeling of multi-component crystallization of industrial-grade oils and fats

Transient crystallization kinetics is investigated for complex, industrial-grade vegetable oils consisting of more than ten triacylglycerols (TAG). The classical nucleation model has been used to describe primary nucleation, while secondary nucleation has been described by a semi-empirical approach. Growth is modeled using a modified Burton-Cabrera-Frank (BCF) model. Surface tensions and growth constants have been determined using focused-beam-reflectance measurements (FBRM). The required adjustable parameters in the model have been fitted to overall crystallization curves obtained by solid-fat content (SFC) measurements for a given oil at different cooling rates and degrees of dilution. The developed model can accommodate more polymorphs simultaneously and performs well with respect to predicting crystallization onset, rate of crystallization and final SFC value. It can also qualitatively describe how higher cooling rates lead to formation of more meta-stable crystals and smaller mean-crystal sizes. The model provides a good starting point for developing more realistic, transient models for TAG crystallization with the ability to accommodate processing conditions and complex chemical compositions. Such a predictive model may provide a powerful tool to screen and optimize oil formulations in industrial processes and allow product developers to evaluate recrystallization events.
transient nitrite accumulation and susceptibility of anaerobic ammonium oxidizing bacteria in systems with size-segregated aggregates, both aerobic and anaerobic ammonium oxidizing guilds, at sufficiently low oxygen to ammonium loadings. However, anaerobic ammonium oxidizing guilds, could achieve removal efficiencies comparable to stratified aggregates (containing the optimal oxygen to ammonium loadings. Size-segregated aggregates consisting of exclusively aerobic or exclusively anaerobic ammonia oxidizing processes. The footprint can be further reduced by process intensification in single-stage reactors. Single-stage reactors can greatly reduce operational energy costs compared to traditional nitrogen removal processes, or services in order to support the selection making of desired products and/or processes from different alternatives. For more sustainable process designs, technical requirements have to be evaluated together with environmental and economic aspects. The LCSOFT software-tool has been developed to perform LCA as a stand-alone tool as well as integrated with other process design tools such as process simulation, economic analysis (ECON), and sustainable process design (SustainPro). An extended version of LCSOFT is presented in this paper. The development work consists of four main tasks. The first task consists of the Life Cycle Inventory (LCI) calculation function. The second task deals with the extension of the Life Cycle Inventory database and improvement of the Life Cycle Impact Assessment calculation. The third task deals with analysis to investigate the contributions of processes, LCI results, and environmental impact results with respect to the production stage. Also, an uncertainty analysis is included to investigate the influence of uncertain parameters on the LCA assessment results. The fourth task has been added to validate and improve LCSOFT by testing it against several case studies and compare the assessment results with other available tools.

Management of microbial community composition, architecture and performance in autotrophic nitrogen removing bioreactors through aeration regimes

Completely autotrophic nitrogen removal from nitrogen-rich wastewaters through the nitritation -plus- anaerobic ammonium oxidation processes can greatly reduce operational energy costs compared to traditional nitrogen removal processes. The footprint can be further reduced by process intensification in single-stage reactors. Single-stage reactors require biofilms or bioaggregates to provide the complementary redox niches for the aerobic and anaerobic bacteria that are required for nitritation and anaerobic ammonium oxidation (anammox), respectively. The nitritation/anammox process might not only reduce aeration and carbon requirements but also reduce emissions of the greenhouse gas nitrous oxide. Successful performance of the intense energy-efficient nitritation/anammox process requires a rather narrow operational window. Outside of this window, disproportionate activities of the involved functional guilds and emergence of undesired guilds can rapidly deteriorate the performance, which will offset the reduced footprint and stability. Hence, robust operational strategies that incorporate microbial process understanding are necessary.

In this work, aeration strategies were systematically evaluated as an approach to manipulate the microbial community structure, to reach efficient nitrogen removal performance, and to reduce nitrous oxide emissions from single-stage nitritation/anammox reactors. First, an iterative protocol was developed to diagnose reactor performance based on process stoichiometry and to propose actions to enhance performance based on discretized aeration parameters, restricted by an overall ratio of oxygen to ammonium loading. The protocol was successfully applied on two bioaggregate-based single-stage sequencing batch reactors during start-up; while recovering from major disturbances such as nitrite accumulation, nitrite oxidizer proliferation, ammonium starvation, and oxygen overloading; and during nitrogen loading increases. Different mitigation methods were validated or falsified ultimately improving the proposed protocol. Differences in performance and, especially, of time resolved nitrogen species dynamics, of the two parallel systems under similar aeration regimes indicated that the aggregate size distribution and microbial community architectures profoundly affected the optimal oxygen to ammonium loadings. Size-segregated aggregates consisting of exclusively aerobic or exclusively anaerobic ammonium oxidizing guilds, could achieve removal efficiencies comparable to stratified aggregates (containing both aerobic and anaerobic ammonium oxidizing guilds), at sufficiently low oxygen to ammonium loadings. However, transient nitrite accumulation and susceptibility of anaerobic ammonium oxidizing bacteria in systems with size-segregated aggregate structures were investigated.
aggregates were considered to weaken the system robustness. Further assessment of the interaction between aeration regime and architectural evolution of the nitritation/anammox aggregates was carried out on the two systems once they achieved steady state overall performance. With settling time, volumetric exchange ratio, sludge retention time and influent characteristics kept constant, the aeration regime, itself, caused changes in aggregate architecture and aggregate size distribution. By increasing aeration frequency, the originally size-segregated community became more redox-stratified with larger aggregates. Increasing the duration of aeration, on the other hand, did not significantly alter the original redox-stratified architecture, but allowed proliferation of unwanted nitrite oxidizing bacteria. The decrease in aeration intensity concomitant with increased duration also decreased the aggregate size. Aggregate morphology and settleability were also altered with aeration regime: increased frequencies led to compact but hollow aggregates that transiently accumulated nitrogen gas. Based on the experimental observations, a conceptual scheme was proposed to describe aggregation and architectural evolution in nitritation/anammox reactors, incorporating the possible influences of intermediates formed with intermittent aeration. Community analysis revealed an abundant fraction of heterotrophic types despite the absence of organic carbon in the feed. The aerobic and anaerobic ammonia oxidizing guilds were dominated by fast-growing Nitrosomonas spp. and Ca. Brocadia spp., while the nitrite oxidizing guild was dominated by high affinity Nitrospira spp.

Emission of nitrous oxide (N2O) was evaluated from both reactors under dynamic aeration regimes. Contrary to the widely held notion that dynamic operation at low dissolved oxygen concentrations would increase nitrous oxide emissions, increasing the aeration frequencies reduced N2O production and emission. N2O production was observed primarily at the onset of aeration after anoxia. Nitric oxide and not free nitrous acid or nitrite correlated to production rates. The measured aerobic ammonia oxidation potential correlated to the nitrous oxide production rates. Shortening the duration of single aerated periods was an efficient way of preventing the exponential increase in N2O production rates. Correspondingly, operating nitritation/anammox reactors under limited aerobic and excess anaerobic ammonia oxidation is recommended to minimize N2O production and emission.

Aeration impacts the nitritation/anammox process in multiple dimensions. This study focused on the different oxygen delivery schemes, and some of the collateral impacts could be isolated, increasing process understanding. It was demonstrated that aeration strategy can be used as a powerful tool to manipulate the microbial community composition, its architecture and reactor performance. We suggest operation via intermittent aeration with short aerated periods to minimize nitrous oxide emission rates and sufficiently long non-aerated periods to suppress nitrite oxidizing bacteria. Under these conditions, redox-stratified aggregates can be established maintaining simultaneously aerobic and anaerobic autotrophic ammonium oxidation in an intensified single-stage reactor.

Nitritation/anammox processes have already been successfully applied to treat side stream reject waters, landfill leachates and industrial wastewater streams; now this process is being examined to replace or upgrade conventional treatment trains to treat domestic wastewaters under low temperatures in the presence of residual organic carbon. This work, by examining the interplay between macro- and micro-scale phenomena and processes, contributes to establishment of strategies that can be adopted in practice to operate the single-stage nitritation/anammox systems.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Mutlu, A. G. (Intern), Smets, B. F. (Intern), Sin, G. (Intern)
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Mathematical modelling of anaerobic digestion processes: applications and future needs
Anaerobic process modelling is a mature and well-established field, largely guided by a mechanistic model structure that is defined by our understanding of underlying processes. This led to publication of the IWA ADM1, and strong supporting, analytical, and extension research in the 15 years since its publication. However, the field is rapidly expanding, in terms of new technology, new processes, and the need to consider anaerobic processes in a much broader context of the wastewater cycle as a whole. Within the area of technologies, new processes are emerging (including high-solids and domestic wastewater treatment). Challenges relating to these new processes, as well as the need to intensify and better operate existing processes have increased the need to consider spatial variance, and improve characterisation of inputs. Emerging microbial processes are challenging our understanding of the role of the central carbon catabolic metabolism in anaerobic digestion, with an increased importance of phosphorous, sulfur, and metals as electron source and sink, and consideration of hydrogen and methane as potential electron sources. The paradigm of anaerobic digestion is challenged by anoxicogenic phototrophism, where energy is relatively cheap, but electron transfer is expensive. These new processes are commonly not compatible with the existing structure of anaerobic digestion models. These core issues extend to
application of anaerobic digestion in domestic plant-wide modelling, with the need for improved characterisation, new technologies having an increased impact, and a key role for the linked phosphorous–sulfur–iron processes across the cycle. The review overall finds that anaerobic modelling is increasing in complexity and demands on the modeller, but the core principles of biochemical and physicochemical processes, metabolic conservation, and mechanistic understanding will serve well to address the new challenges.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Queensland, Universidad Rey Juan Carlos, Masdar Institute of Science and Technology
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Scopus rating (2015): SJR 1.233 SNIP 1.846 CiteScore 3.96
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Scopus rating (2014): SJR 1.245 SNIP 1.806 CiteScore 3.42
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 0.941 SNIP 1.192 CiteScore 2.07
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.167 SNIP 1.753 CiteScore 2.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.16 SNIP 1.449
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.955 SNIP 1.796
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Scopus rating (2008): SJR 0.858 SNIP 1.295
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Scopus rating (2006): SJR 0.588 SNIP 0.7
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**Method for innovative synthesis-design of chemical process flowsheets**

Chemical process synthesis-design involve the identification of the processing route to reach a desired product from a specified set of raw materials, design of the operations involved in the processing route, the calculations of utility requirements, the calculations of waste and emission to the surrounding and many more. Different methods (knowledge-based [1], mathematical programming [2], hybrid, etc.) have been proposed and are also currently employed to solve these synthesis-design problems. D’Anterroches [3] proposed a group contribution based approach to solve the synthesis-design problem of chemical processes, where, chemical process flowsheets could be synthesized in the same way as atoms or groups of atoms are synthesized to form molecules in computer aided molecular design (CAMD) techniques [4]. That, from a library of building blocks (functional process-groups) and a set of rules to join them, chemical process flowsheets are generated and evaluated for properties like energy consumption, atom efficiency, environmental impact, etc., using functional process-group based property models. In this way, a list of feasible chemical process flowsheets are quickly generated, screened and selected for further analysis. In the next stage, the design parameters for the operations of the flowsheet are established through reverse engineering approaches based on driving forces available for each operation. In the final stage, when all the necessary information for a rigorous process simulation is available, rigorous simulation is performed to validate the synthesis-design. Note that since the flowsheet is synthesized and the operations in the flowsheet designed to match a set of design targets, there are no iterations involved as the final flowsheet is among the best, if not the best.

In this paper, the implementation of the computer-aided process-group based flowsheet synthesis-design framework is presented together with an extended library of flowsheet property models to predict the environmental impact, safety factors, product recovery and purity, which are employed to screen the generated alternatives. Also, new process groups are added to represent unit operations for applications in bio-processes. The implemented framework in the form of a new computer-aided tool in ICAS (Integrated Computer Aided System) will be highlighted through two case studies, one involving the synthesis of a chemical process flowsheet (the well-known Hydrodealkylation of toluene process) and another for a biochemical process flowsheet (production of ethanol from lignocellulose). In both cases, not only the reported designs are found and matched, but also new innovative designs are found, which is possible because of the predictive nature of the models used and the synthesis of flowsheets through the group contribution approach. The case studies and others developed to test the method, the framework and the ICAS-tool help to confirm their applicability, scope and significance, since it is possible to find new and better alternatives not reported earlier. The application-examples also focus on the use of SFILES notation system, developed specially for the process-group based synthesis-design method, to store and/or visualize the structural information of any process flowsheet represented by process-groups. As an extension, the SFILES notation is extended to store the process information through which representation of flowsheet alternatives for rigorous process simulation (for example, with an external process simulator) would be possible.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium
Authors: Kumar Tula, A. (Intern), Gani, R. (Intern)
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**Methods and tools for sustainable chemical process design**

As the pressure on chemical and biochemical processes to achieve a more sustainable performance increases, the need to define a systematic and holistic way to accomplish this is becoming more urgent. In this chapter, a multilevel computer-aided framework for systematic design of more sustainable chemical processes is presented. The framework allows the use of appropriate computer-aided methods and tools in a hierarchical manner according to a developed work flow for a multilevel criteria analysis that helps generate competing and more sustainable process design options. The application of the framework as well as the related computer-aided methods and tools are highlighted through a case study involving the production of bioethanol from various renewable raw materials.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Chulalongkorn University
Authors: Loureiro da Costa Lira Gargalo, C. (Intern), Chairakwongsa, S. (Ekstern), Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Microscale technology and biocatalytic processes: Opportunities and challenges for synthesis
Despite the expanding presence of microscale technology in chemical synthesis and energy production as well as in biomedical devices and analytical and diagnostic tools, its potential in biocatalytic processes for pharmaceutical and fine chemicals, as well as related industries, has not yet been fully exploited. The aim of this review is to shed light on the strategic advantages of this promising technology for the development and realization of biocatalytic processes and subsequent product recovery steps, demonstrated with examples from the literature. Constraints, opportunities, and the future outlook for the implementation of these key green engineering methods and the role of supporting tools such as mathematical models to establish sustainable production processes are discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Sigma-Aldrich Chemie GmbH, University of Ljubljana
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Scopus rating (2016): CiteScore 9.97 SJR 4.037 SNIP 3.143
BFI (2015): BFI-level 2
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Model-Based Analysis and Efficient Operation of a Glucose Isomerization Reactor Plant

The application of computer-aided model based methods within an integrated systematic framework is illustrated with the objective to assist the multi-purpose pharmaceutical/biochemical industry to systematically solve the complex problems that are experienced when aiming at improving the process efficiency. The objective of this study is the application of the developed framework on an industrial case study of a glucose isomerization (GI) reactor plant that is part of a corn refinery, with the objective to improve the productivity of the process. Therefore, a multi-scale reactor model is developed for use as a building block for the GI reactor plant simulation. An optimal operation strategy is proposed on the basis of the simulation results.

General information
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Model-based characterisation of twin-screw granulation system for continuous solid dosage manufacturing

Since large molecules are considered the key driver for growth of the pharmaceutical industry, the focus of the pharmaceutical industry is shifting from small molecules to biopharmaceuticals: around 50% of the approved biopharmaceuticals are freeze-dried products. Therefore, freeze-drying is an important technology to stabilise biopharmaceutical drug products which are unstable in an aqueous solution. However, the freeze-drying process is an energy and time-consuming process. The use of mechanistic modelling to gather process knowledge can assist in optimisation of the process parameters during the operation of the freeze-drying process. By applying a dynamic shelf temperature and chamber pressure, which are the only controllable process variables, the processing time can be decreased by a factor 2 to 3.

Model-based optimization of the primary drying step during freeze-drying

Since large molecules are considered the key driver for growth of the pharmaceutical industry, the focus of the pharmaceutical industry is shifting from small molecules to biopharmaceuticals: around 50% of the approved biopharmaceuticals are freeze-dried products. Therefore, freeze-drying is an important technology to stabilise biopharmaceutical drug products which are unstable in an aqueous solution. However, the freeze-drying process is an energy and time-consuming process. The use of mechanistic modelling to gather process knowledge can assist in optimisation of the process parameters during the operation of the freeze-drying process. By applying a dynamic shelf temperature and chamber pressure, which are the only controllable process variables, the processing time can be decreased by a factor 2 to 3.
Modeling and analysis of conventional and heat-integrated distillation columns

A generic model that can cover diabatic and adiabatic distillation column configurations is presented, with the aim of providing a consistent basis for comparison of alternative distillation column technologies. Both a static and a dynamic formulation of the model, together with a model catalogue consisting of the conventional, the heat-integrated and the mechanical vapor recompression distillation columns are presented. The solution procedure of the model is outlined and illustrated in three case studies. One case study being a benchmark study demonstrating the size of the model and the static properties of two different heat-integrated distillation column (HIDiC) schemes and the mechanical vapor recompression column. The second case study exemplifies the difference between a HIDiC and a conventional distillation column in the composition profiles within a multicomponent separation, whereas the last case study demonstrates the difference in available dynamic models for the HIDiC and the proposed model.
Heat-integrated distillation column, Diabatic, Distillation, Heat integration, Simulation

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Modeling Mass Transfer in Small Scale Reactors Using Computational Fluid Dynamics

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Authors: Larsson, H. (Intern), Gernaey, K. (Intern), Krühne, U. (Intern)
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Modeling the Automotive SCR Catalyst

General information
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Modelling of Mass Transfer Phenomena in Chemical and Biochemical Reactor Systems using Computational Fluid Dynamics

Computational fluid dynamics (CFD) is the application of numerical methods to solve systems of partial differential equations related to fluid dynamics. The continuity and the momentum equations are the most commonly applied equations within CFD, and together they can be used to calculate the velocity and pressure distributions in a fluid. CFD also enables the modelling of several fluids simultaneously, e.g. gas bubbles in a liquid, as well as the presence of turbulence and dissolved chemicals in a fluid, and many other phenomena. This makes CFD an appreciated tool for studying flow structures, mixing, and other mass transfer phenomena in chemical and biochemical reactor systems.

In this project, four selected case studies are investigated in order to explore the capabilities of CFD. The selected cases are a 1 ml stirred microbioreactor, an 8 ml magnetically stirred reactor, a Rushton impeller stirred pilot plant reactor, and a rotating bed reactor filled with catalytic porous material. A selection of the simulated phenomena includes the velocities and turbulent quantities in the reactors, as well as the distribution of the gas and liquid phases in them. Mixing times, oxygen transfer rates and an ion-exchange reaction are also modelled and compared to experimental data.

The thesis includes a comprehensive overview of the fundamentals behind a CFD software, as well as a more detailed review of the fluid dynamic phenomena investigated in this project. The momentum and continuity equations are presented as well as the theory behind the SST and the k-ε turbulence models. Modelling of additional variables, porous materials and two-phase flows are also introduced. The two-phase flows are modelled using the Euler-Euler method, and both dispersed and free-surface flows are simulated.

The importance of mass transfer with a focus on mixing, gas-liquid transfer of oxygen, and heterogeneous reactor systems is reviewed and mathematical models for these applications are presented. A review of how these mass transfer phenomena have been modelled in the scientific literature is also included.

The models are subsequently evaluated based on their applicability in the four case studies. The evaluations especially focus on the impact of the choice of turbulence model and other modelling decisions made by the user. The conclusion is that CFD is a highly valuable tool for modelling several important parameters in chemical and biochemical reactors but that the user must be well aware of the shortcomings with the applied models.
Modelling of phase equilibria and related properties of mixtures involving lipids

Many challenges involving physical and thermodynamic properties in the production of edible oils and biodiesel are observed, such as availability of experimental data and reliable prediction. In the case of lipids, a lack of experimental data for pure components and also for their mixtures in open literature was observed, what makes it necessary to develop reliable predictive models from limited data. One of the first steps of this project was the creation of a database containing properties of mixtures involved in tasks related to process design, simulation, and optimization as well as design of chemicals based products. This database was combined with the existing lipids database of pure component properties. To contribute to the missing data, measurements of isobaric vapour-liquid equilibrium (VLE) data of two binary mixtures at two different pressures were performed using Differential Scanning Calorimetry (DSC) technique. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC model and by proposing new interaction parameters for original UNIFAC model and lipids systems. Available thermodynamic consistency tests were applied before performing parameter regressions for well-known thermodynamic models such as NRTL, UNIQUAC and original UNIFAC. The performance of the excess Gibbs energy (GE) based models was also evaluated for lipids data and the fitted parameters contributed to the extension of the created database. The consistency of the available VLE data has been checked using a general and robust approach developed by the Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST). For SLE data, consistency tests based on the Gibbs–Duhem equation are not feasible, thus in this project new consistency tests have been developed. Moreover, a methodology that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions is discussed. The SLE consistency test and data evaluation is performed in a software containing options for data analysis, model analysis and parameter regression.

Modelling phosphorus (P), sulphur (S) and iron (Fe) interactions during the simulation of anaerobic digestion processes

This paper examines the effects of different model formulations when describing sludge stabilization processes in wastewater treatment plants by the Anaerobic Digestion Model No. 1 (ADM1). The proposed model extensions describe the interactions amongst phosphorus (P), sulfur (S), iron (Fe) and their potential effect on total biogas production (CO2, CH4, H2 and H2S). 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). Four (A1 – A4) different model extensions are implemented, simulated and evaluated. The first approach (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). The second model formulation (A2) describes biological production of sulfide (SH2S) by means of Sulfate-Reducing Bacteria (XSRB). This approach also considers potential SH2S inhibition effect on biomass and mass transfer phenomena (aqueous-gas). The third evaluated model (A3) considers chemical iron (III) (SP+3) reduction to iron (II) (SP+2) using hydrogen (H2) as the electron donor. Finally, the last evaluated approach (A4) is based on accounting for Multiple Mineral Precipitation. The ADM1 thereby switches from a 2-phase (aqueous-gas) to a 3-phase (aqueous-gas-solid) system. Simulation results show that the implementations of A1, A2 and A3 lead to a reduction in biogas production. This reduction is attributed to two factors. Firstly, there is a fierce competition for substrate (S, H2, VFA) between the existing and the new groups of microorganisms. Secondly, there is a decrease of acetilastic and hydrogenotrophic methanogenesis due to SH2S inhibition. Models A3 and A4 reduce the free SH2S (and consequently inhibition) plus cationic load and soluble P availability due to ion pair formation and metallic carbonate/phosphate precipitation. The final version of the manuscript will provide a deeper analysis of the different model assumptions, the effect that operational/design conditions might have on the model predictions, a detailed description of the weak acid-base chemistry and practical implications in view of plant-wide modelling/development of resource recovery strategies.

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Multivariate analysis of industrial scale fermentation data

Batch production processes pose specific challenges for process monitoring and control. This is due to many reasons including non-linear behaviour, and a relatively poor understanding of the system dynamics. It is therefore challenging for the process engineer to optimise the operation conditions, due to a lack of available process models, and complex interactions between variables which are not easy to define, especially across scales and equipment. There is however a vast amount of batch process data generated, which can be investigated with the aim of identifying desirable process operating conditions, and therefore areas of focus for optimising the process operation. This requires multivariate methods which can utilise the complex datasets which are routinely collected, containing online measured variables and offline sample data.

Fermentation processes are highly sensitive to operational changes, as well as between batch variations, and are therefore an interesting application of multivariate methods. The process dynamics are governed by the combination of process variables, and cannot be fully characterised by individual variables alone. There is also a lack of sensors for key variables which are considered to define the operation, which makes traditional modelling a challenge. Although multivariate techniques are routinely used for chemometric applications, their application to batch processes is less common due to the additional challenges associated with uneven batch lengths and less reproducible data, which has naturally greater variability, as well as higher measurement noise. This requires additional preprocessing stages in order to extract the information within such a dataset.

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. By creating a model for product concentration, it is possible to analyse the model results and interpret this to guide process optimisation efforts towards achieving a greater product concentration.
Novel strategies for control of fermentation processes

Bioprocesses are inherently sensitive to fluctuations in processing conditions and must be tightly regulated to maintain cellular productivity. Industrial fermentations are often difficult to replicate across production sites or between facilities as the small operating differences in the equipment affect the way the batches should be optimally run. In addition, batches run in the same facility can also be affected by batch variations in the growth characteristics of a specific cultivation. There is demand therefore to identify key monitoring parameters and to continually monitor the performance of a fermentation.

Industrial fermentation processes are typically operated in fed batch mode, which also poses specific challenges for process monitoring and control. This is due to many reasons including non-linear behaviour, and a relatively poor understanding of the system dynamics. It is therefore challenging for the process engineer to optimise the operation conditions, due to a lack of available process models, and complex interactions between variables which are not easy to define, especially across scales and equipment. There is however a vast amount of batch process data generated, which can be investigated with the aim of identifying desirable process operating conditions, and therefore areas of focus for optimising the process operation. This requires multivariate methods which can utilise the complex datasets which are routinely collected, containing online measured variables and offline sample data. This is interesting, since the process dynamics are governed by the combination of process variables, and cannot be fully characterised by individual variables alone.

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. By creating a model for product concentration, it is possible to analyse the model results and interpret this to guide process optimisation efforts towards achieving a greater product concentration. By analysis of the variable contributions to the prediction, and the variable trends, it may be possible to develop improved control strategies for these variables.
Optimal Design of Algae Biorefinery Processing Networks for the production of Protein, Ethanol and Biodiesel

In this study, optimal design of algal biorefinery using microalgae with respect to techno-economic criteria is studied. A systematic methodology using superstructure-based optimization is used to this end. A superstructure representing a wide range of technologies developed for processing microalgae to produce end products is formulated. The corresponding technical and economic data is collected and structured using a generic input-output mass balance models. An optimization problem is formulated and solved to identify the optimal designs. The effect of uncertainties inherent in economic analysis such as microalgae production cost, composition of microalgae (e.g. oil content) and biodiesel/bioethanol market prices is considered. New optimal processing paths are found with potential of producing higher amount of biodiesel. Last, the methodology is intended as decision support tool for early-stage concept screening to enhance the future development of algal biorefinery.

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Optimal design of microalga-based biorefinery: Economics, opportunities and challenges

Microalgae have great potential as a feedstock for the production of a wide range of end-products under the broad concept of biorefinery. In an earlier work, we proposed a superstructure based optimization model to find the optimal processing pathway for the production of biodiesel from microalgal biomass, and identified several challenges with the focus being on utilizing lipids extracted microalgal biomass for economic and environmentally friendly production of useful energy products. In this paper, we expand the previous optimization framework by considering the processing of microalgae residue previously treated as wastes. We develop an expanded biorefinery superstructure model, based on which a mixed integer nonlinear programming (MINLP) model is proposed to determine the optimal/promising biorefinery configurations with different choices of objective functions. The MINLP model is solved in GAMS using a database built in Excel. Economic sensitivity analysis is performed to elaborate the potential improvements in the overall economics, and set the targets that must be achieved in the future in order for microalgal biofuels to become economically viable.

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Optimal processing pathway selection for microalgae-based biorefinery under uncertainty

We propose a systematic framework for the selection of optimal processing pathways for a microalgaebased biorefinery under techno-economic uncertainty. The proposed framework promotes robust decision making by taking into account the uncertainties that arise due to inconsistencies among and shortage in the available technical information. A stochastic
mixed integer nonlinear programming (sMINLP) problem is formulated for determining the optimal biorefinery
configurations based on a superstructure model where parameter uncertainties are modeled and included as sampled
scenarios. The solution to the sMINLP problem determines the processing technologies, material flows, and product
portfolio that are optimal with respect to all the sampled scenarios. The developed framework is implemented and tested
on a specific case study. The optimal processing pathways selected with and without the accounting of uncertainty are
compared with respect to different objectives. (C) 2015 Elsevier Ltd. All rights reserved.

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Web of Science (2008): Indexed yes
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Optimization-based methodology for wastewater treatment plant synthesis – a full scale retrofitting case study

Existing wastewater treatment plants (WWTP) need retrofitting in order to better handle changes in the wastewater flow and composition, reduce operational costs as well as meet newer and stricter regulatory standards on the effluent discharge limits. In this study, we use an optimization based framework to manage the multi-criteria WWTP design/retrofit problem for domestic wastewater treatment. The design space (i.e. alternative treatment technologies) is represented in a superstructure, which is coupled with a database containing data for both performance and economics of the novel alternative technologies. The superstructure optimization problem is formulated as a Mixed Integer (non)Linear Programming problem and solved for different scenarios - represented by different objective functions and constraint definitions. A full-scale domestic wastewater treatment plant (265,000 PE) is used as a case study in order to highlight the use of the framework for generating optimal retrofitting solutions.

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Outlier treatment for improving parameter estimation of group contribution based models for upper flammability limit

Flammability data is needed to assess the risk of fire and explosions. This study presents a new group contribution (GC) model to predict the upper flammability limit UFL oforganic chemicals. Furthermore, it provides a systematic method for outlier treatment inorder to improve the parameter estimation of the GC model. The new method identifies and removes outliers based on the empirical cumulative distribution plot. It is compared to outlier detection based on Cook’s distance and normal cumulative distribution.

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Oxygen transfer rates and requirements in oxidative biocatalysis

Biocatalytic oxidation reactions offer several important benefits such as regio- and stereoselectivity, avoiding the use of toxic metal based catalysts and replacing oxidizing reagents by allowing the use of oxygen. However, the development of biocatalytic oxidation processes is a complex task which requires simultaneous consideration of several issues regarding the process design and operation. In this work, the oxygen requirements are analysed for different process scenarios, considering different biocatalyst formats and variation of the desired productivity. Also, the applicability of two different oxygen supply methods (bubbling and membrane aeration) investigated. Hollow fibre membrane contactors present an interesting alternative for reactor aeration, creating large specific areas (area/volume) of the gas/liquid interface. The modular design of membrane contactors, scaling-up is relatively straightforward (Gabelman and Hwang, 1999), and membrane contactors are implemented for various industrial applications (Klaassen et al., 2005).

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Oxygen transfer rates and requirements in oxidative biocatalysis

Biocatalytic oxidation reactions offer several important benefits such as regio- and stereoselectivity, avoiding the use of toxic metal based catalysts and replacing oxidizing reagents by allowing the use of oxygen. In this contribution the oxygen requirements are analysed for different process scenarios, considering different biocatalyst formats and variation of the desired productivity. Also, the applicability of two different oxygen supply methods (bubbling and membrane aeration) investigated. Hollow fibre membrane contactors present an interesting alternative for reactor aeration, creating large specific areas (area/volume) of the gas/liquid interface. The modular design of membrane contactors, scaling-up is relatively straightforward (Gabelman and Hwang, 1999), and membrane contactors are implemented for various industrial applications (Klaassen et al., 2005).

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Population balance models: a useful complementary modelling framework for future WWTP modelling

Population balance models (PBMs) represent a powerful modelling framework for the description of the dynamics of properties that are characterised by distributions. This distribution of properties under transient conditions has been demonstrated in many chemical engineering applications. Modelling efforts of several current and future unit processes in wastewater treatment plants could potentially benefit from this framework, especially when distributed dynamics have a significant impact on the overall unit process performance. In these cases, current models that rely on average properties cannot sufficiently capture the true behaviour and even lead to completely wrong conclusions. Examples of distributed properties are bubble size, floc size, crystal size or granule size. In these cases, PBMs can be used to develop new knowledge that can be embedded in our current models to improve their predictive capability. Hence, PBMs should be regarded as a complementary modelling framework to biokinetic models. This paper provides an overview of current applications, future potential and limitations of PBMs in the field of wastewater treatment modelling, thereby looking over the fence to other scientific disciplines.

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Web of Science (2006): Indexed yes
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Web of Science (2005): Indexed yes
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Process Alternatives for Second Generation Ethanol Production from Sugarcane Bagasse

In ethanol production from sugarcane juice, sugarcane bagasse is used as fuel for the boiler, to meet the steam and electric energy demand of the process. However, a surplus of bagasse is common, which can be used either to increase electric energy or ethanol production. While the first option uses already established processes, there are still many uncertainties about the techno-economic feasibility of the second option. In this study, some key parameters of the second generation ethanol production process were analyzed and their influence in the process feasibility assessed. The simulated process includes the enzymatic hydrolysis of sugarcane bagasse pretreated with liquid hot water, and the analyzed parameters were the solid consistency in the hydrolysis and pretreatment reactors and the hydrolysis reaction time. The solid consistency in the hydrolysis reactor had the highest influence on the economic feasibility of the process. For the economic scenario considered in this study, using bagasse to increase ethanol production yielded higher ethanol production costs compared to using bagasse for electric energy production, showing that further improvements in the process are still necessary.
Process considerations for use of galactose oxidase as an industrial biocatalyst

In nature galactose oxidase (GOase, EC.1.1.3.9) catalyses the oxidation of the C6 hydroxyl group of D-galactose to the corresponding aldehyde, while reducing molecular oxygen to hydrogen peroxide. In recent years a great effort has been made to broaden the substrate scope, enabling GOase to oxidize C6-OH of glucose and fructose, as well as secondary alcohols to ketones. The widened substrate scope of GOase opens up many important industrial applications, such as synthesis of industrially relevant compounds containing aldehydes and ketones (e.g. the oxidation of 5-hydroxymethylfurfural to diformylfuran), deracemization of secondary alcohols, and modification of a wide range of naturally occurring polysaccharides [1,2]. Despite these promising characteristics of GOase, application at industrial scale has not been achieved so far. This can in part be ascribed to the process challenges experienced when performing oxidative biocatalysis at a large scale.

Process development for the production of 15β-hydroxycyproterone acetate using Bacillus megaterium expressing CYP106A2 as whole-cell biocatalyst

Background: CYP106A2 from Bacillus megaterium ATCC 13368 was first identified as a regio- and stereoselective 15 beta-hydroxylase of 3-oxoΔ4-steroids. Recently, it was shown that besides 3-oxo-Δ4-steroids, 3-hydroxy-Δ5-steroids as well as di- and triterpenes can also serve as substrates for this biocatalyst. It is highly selective towards the 15β position, but the 6 β, 7 a/β, 9a, 11a and 15a positions have also been described as targets for hydroxylation. Based on the broad substrate spectrum and hydroxylating capacity, it is an excellent candidate for the production of human drug metabolites and drug precursors.

Results: In this work, we demonstrate the conversion of a synthetic testosterone derivative, cyproterone acetate, by CYP106A2 under in vitro and in vivo conditions. Using a Bacillus megaterium whole-cell system overexpressing CYP106A2, sufficient amounts of product for structure elucidation by nuclear magnetic resonance spectroscopy were obtained. The product was characterized as 15β-hydroxyacyproterone acetate, the main human metabolite. It is highly selective towards the 15β position, but the 6 β, 7 a/β, 9a, 11a and 15a positions have also been described as targets for hydroxylation. Based on the broad substrate spectrum and hydroxylating capacity, it is an excellent candidate for the production of human drug metabolites and drug precursors.

Conclusions: Here we describe the successful scale-up of cyproterone acetate conversion from shake flasks to bioreactors, using the CYP106A2 enzyme in a whole-cell system. The substrate was converted to its main human metabolite, 15 β-hydroxyacyproterone acetate, a highly interesting drug candidate, due to its retained antiandrogen activity.
but significantly lower progestogen properties than the mother compound. Optimization of the process led to an
improvement from 55% to 98% overall conversion, with a product formation of 0.43 g/L, approaching industrial process
requirements and a future large-scale application.
Process Intensification Tools in the Small-Scale Pharmaceutical Manufacturing of Small Molecules

The chemical process industry is paying significant attention to the intensification of processes with the main aim of achieving increased productivity, improved economic status, and enhanced sustainability. The pharmaceutical industry is moving in the same direction and, therefore, dozens of processes are in a state of change. However, it is important to note that not all processes can be intensified easily, such as slow chemical reactions, processes with solids, slurries, and on the like. This review summarizes applications of promising tools for achieving process intensification in the small-scale pharmaceutical manufacturing of so-called small molecules. The focus is on microwave radiation, microreactors, ultrasounds, and meso-scale tubular reactors.

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Biocatalytic oxidation reactions have the potential to substitute many chemically catalyzed oxidations in the pharmaceutical and fine chemical industry due to their superior regio- and stereoselectivity and low environmental impact. Galactose oxidase (GOase) has been shown to be a promising biocatalyst for the oxidation of primary and secondary alcohols to their corresponding aldehydes and ketones, respectively. However, GOase requires a number of additives to sustain its catalytic function, such as the enzyme catalase for degradation of the byproduct hydrogen peroxide as well as single-electron oxidants to reactivate the enzyme upon loss of the amino acid radical in its active site. In this work, the addition of catalase, single-electron oxidants, and copper ions was investigated systematically in order to find the minimum concentrations required to obtain a fully active GOase. Furthermore, it was found that the concentration and type of buffer is essential for the activity of GOase, which was significantly more active in sodium phosphate buffer than in other buffers investigated. Enzyme stability and oxygen requirements are of crucial importance for the implementation of oxidase based processes. GOase was shown to be completely stable for 120 h in buffer with stirring at 25 °C, and the activity even increased 30% if the enzyme solution was also aerated in a similar experiment. The high $K_m$ for oxygen of GOase (>5 mM) relative to the solubility of oxygen in water reveals a trade-off between supplying oxygen at a sufficiently high rate and ensuring a high degree of enzyme utilization (i.e., ensuring the highest possible specific rate of reaction). Nevertheless, the good stability and high activity of GOase bode well for its future application as an industrial biocatalyst.
**Process synthesis, design and analysis using a process-group contribution method**

This paper describes the development and application of a process-group contribution method to model, simulate and synthesize chemical processes. Process flowsheets are generated in the same way as atoms or groups of atoms are combined to form molecules in computer aided molecular design (CAMD) techniques. The fundamental pillars of this framework are the definition and use of functional process-groups (building blocks) representing a wide range of process operations, flowsheet connectivity rules to join the process-groups to generate all the feasible flowsheet alternatives and flowsheet property models like energy consumption, atom efficiency, environmental impact to evaluate the performance of the generated alternatives. In this way, a list of feasible flowsheets are quickly generated, screened and selected for further analysis. Since the flowsheet is synthesized and the operations in the flowsheet designed through predictive models to match a set of design targets, optimal solution of a given synthesis problem is guaranteed. (C) 2015 Elsevier Ltd. All rights reserved.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Auburn University  
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BFI (2010): BFI-level 2  
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Product design - Molecules, devices, functional products, and formulated products

Chemical product design is a multidisciplinary and diverse subject. This article provides an overview of product design while focusing on product conceptualization. Four product types are considered - molecular products, formulated products, devices and functional products. For molecular products, computer-aided design tools are used to predict the physicochemical properties of single molecules and blends. For formulated products, an integrated experiment-modeling approach is used to generate the formula with the specified product attributes. For devices and functional products, conceptual product design is carried out by modeling the product based on thermodynamics, kinetics and transport processes, by performing experiments, and by decision making based on rule-based methods. The results are product specifications in terms of the type of ingredients, composition, and the structure, form, shape or configuration of the product.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Hong Kong University of Science and Technology
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Real-Time Model Based Process Monitoring of Enzymatic Biodiesel Production

In this contribution we extend our modelling work on the enzymatic production of biodiesel where we demonstrate the application of a Continuous-Discrete Extended Kalman Filter (a state estimator). The state estimator is used to correct for mismatch between the process data and the process model for Fed-batch production of biodiesel. For the three process runs investigated, using a single tuning parameter, \( q_x = 2 \times 10^{-2} \) which represents the uncertainty in the process model, it was possible over the entire course of the reaction to reduce the overall mean and standard deviation of the error between
the model and the process data for all of the five measured components (triglycerides, diglycerides, monoglycerides, fatty acid methyl esters, and free fatty acid). The most significant reduction for the three process runs, were for the monoglyceride and free fatty acid concentration. For those components, there was over a ten-fold decrease in the overall mean error for the state estimator prediction compared with the predictions from the pure model simulations. It is also shown that the state estimator can be used as a tool for detection of outliers in the measurement data. For the enzymatic biodiesel process, given the infrequent and sometimes uncertain measurements obtained we see the use of the Continuous-Discrete Extended Kalman Filter as a viable tool for real time process monitoring.

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Regulatory control analysis and design for sewer systems

A systematic methodology for regulatory control analysis and design is adapted for sewer system operation and evaluated. The main challenge with adapting the methodology is the handling of the stochastic and transient nature of the rainfall disturbances, inherent to sewer system operation. To this end, four distinct modes of operation are identified (dry weather, filling, saturation and emptying) and for each of these the process gain matrix is found. Based on the gain matrices a controllability analysis is performed, to screen for suitable pairings between measurements and actuators in the case study area of Copenhagen. The analysis effectively reduces the number of potential controlled variables, by considering the sensitivity of the measurements towards changes in the manipulated variables. Several potential pairings are generated and the best alternative is chosen for closed-loop testing. The methodology is a promising tool for systematic generation of solutions for sewer system control.

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Representation and validation of liquid densities for pure compounds and mixtures

Reliable correlation and prediction of liquid densities are important for designing chemical processes at normal and elevated pressures. A corresponding-states model from molecular theory was extended to yield a robust method for quality testing of experimental data that also provides predicted values at unmeasured conditions. The model has been shown to successfully represent and validate the pressure and temperature dependence of liquid densities greater than 1.5 of the critical density for pure compounds, binary mixtures, and ternary mixtures from the triple to critical temperatures at pressures up to 106 kPa. The systems include the full range of organic compounds, including complex solutions, and ionic liquids. Minimal data are required for making predictions.

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**Representation and Validation of Liquid Densities for Pure Compounds and Mixtures**

Reliable correlation and prediction of liquid densities are important for designing chemical processes at normal and elevated pressures. We have extended a corresponding states model from molecular theory to yield a robust method for quality testing of experimental data that also provides predicted values at unmeasured conditions. The model has been shown to successfully validate and represent the pressure and temperature dependence of liquid densities greater than 1.5 of the critical density for pure compounds, binary mixtures, and ternary mixtures from the triple to critical temperatures at pressures up to 1000 MPa. The systems include the full range of organic compounds, including complex mixtures, and ionic liquids. Minimal data are required for making predictions. The presentation will show the implementation of the method, criteria for its deployment, examples of its application to a wide variety of systems over great ranges of conditions, and considerations of further developments.

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**Responses of azeotropes and relative volatilities to pressure variations**

Mixtures with azeotropes cannot be separated by simple distillation since the vapor and liquid compositions are the same. One option to overcome this limitation is to vary the applied pressure to shift the azeotropic composition out of the range of a single column or use pressure-swing operation of two columns. Because operating costs are highly sensitive to the pressure dependence of azeotropic compositions, reliable and accurate phase equilibrium thermodynamic property information is needed to computationally explore pressure variation for such processes. An analysis of property modeling has been done for the pressure sensitivity of azeotropic composition, and examples are given of modeling strategies for binary and ternary mixtures. A quantitative criterion for the need to consider nonideality effects in both modeling and parameter regression has been established, based on similarity of mixture excess enthalpies and pure component enthalpies of vaporization.

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Rules for biocatalyst and reaction engineering to implement effective, NAD(P)H-dependent, whole cell bioreductions

Access to chiral alcohols of high optical purity is today frequently provided by the enzymatic reduction of precursor ketones. However, bioreductions are complicated by the need for reducing equivalents in the form of NAD(P)H. The high price and molecular weight of NAD(P)H necessitate in situ recycling of catalytic quantities, which is mostly accomplished by enzymatic oxidation of a cheap co-substrate. The coupled oxidoreduction can be either performed by free enzymes in solution or by whole cells. Reductase selection, the decision between cell-free and whole cell reduction systems, coenzyme recycling mode and reaction conditions represent design options that strongly affect bioreduction efficiency. In this paper, each option was critically scrutinized and decision rules formulated based on well-described literature examples. The development chain was visualized as a decision-tree that can be used to identify the most promising route towards the production of a specific chiral alcohol. General methods, applications and bottlenecks in the set-up are presented and key experiments required to "test" for decision-making attributes are defined. The reduction of o-chloroacetophenone to (S)-1-(2-chlorophenyl)ethanol was used as one example to demonstrate all the development steps. Detailed analysis of reported large-scale bioreductions identified product isolation as a major bottleneck in process design.
Decision tree for bioreduction development, Design of Escherichia coli whole cell catalysts, Limitations of whole cell reductions, Cost analysis, Scale-up, Chiral alcohol
Sensitivity analysis of Computer-aided molecular design problem for the development of novel working fluids for power cycles

In recent years there is a large availability of low-temperature heat sources in different applications such as waste heat in chemical industries and refrigeration plants as well as renewable energy sources such as biomass combustion, geothermal and solar heat sources. Power cycles are an important technical tool to convert this waste heat into usable energy. So far the low-temperature heat cannot be utilized efficiently for electricity generation. In order to optimize the heat transfer process and the power generation, the influence of the working fluid, the cycle designs and the operating conditions is vital. Multi-criteria database search and Computer Aided Molecular Design (CAMD) can be applied to generate, test and evaluate promising pure component/mixture candidate as process fluids to help optimize cycle design and performance.

The problem formulation for the development of novel working fluids is an advanced CAMD challenge both in terms of data and computational demand, because includes process related as well as property related equations. In CAMD problems the identification of target properties is often based on expert knowledge. To support identification of relevant target properties, in this study, we propose the use of sensitivity analysis. The sensitivity analysis, among others, provides information concerning the influence of a certain property of a candidate working fluid on the performance of the power cycle, i.e. the net power output in this particular application. This information allows the ranking of significance of properties and also the identification of a set of properties which are relevant for the design of a working fluids. In this study the CAMD problem for the development of novel working fluids for organic Rankine cycles (ORC) is formulated as a mathematical optimization problem. It integrates both a system model for the ORC and property models, such as GC+-based models for estimation of pure component properties, Peng-Robinson equation of state for estimation of enthalpy, entropy, etc. The system consists of coupled mass and energy balances for a pump, a condenser, a turbine and an evaporator. A global sensitivity analysis is performed to determine which input parameters (e.g. properties of working fluids, cycle design parameters, etc) have important effects on the net power output. To this end, two methods have been used namely Monte Carlo based linear regression (so called SRC method) as well as Morris Screening techniques. The application of two global sensitivity analysis methods is highlighted for a case study involving power-cycle design forenergy recovery from low-temperature water streams. Temperature 120°C and pressure 4 bar. Overall this contribution presents a new approach for the systematic identification of target properties of CAMD problems based on sensitivity analysis which is validated for the development of novel working fluids of organic Rankine cycles for low temperature heat sources.

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Sensitivity analysis of molecular design problem for the development of novel working fluids for power cycles

In recent years there is a large availability of low-temperature heat sources in different applications such as waste heat in chemical industries and refrigeration plants as well as renewable energy sources such as biomass combustion, geothermal and solar heat sources. Power cycles are an important technology to convert such waste heat sources into usable energy. So far the low-temperature heat is not utilized efficiently for electricity generation.

To optimize the heat transfer process and the power generation, the influence of the working fluid, the cycle designs and the operating conditions is vital. Multi-criteria database search and Computer Aided Molecular Design (CAMD) can be applied to generate, test and evaluate promising pure component/mixture candidate as process fluids to help optimize cycle design and performance [1]. The problem formulation for the development of novel working fluids is a CAMD challenge both in terms of data and computational demand, because includes process related as well as property related equations.
In CAMD problems the identification of target properties is often based on expert knowledge. However, sophisticated information concerning the influence of for example a certain working fluid property parameter on the performance of the power cycle, i.e. the net power output, can facilitate the identification of key properties for working fluids. In that sense a sensitivity analysis of the different parameters is suggested in this work as a systematic method to efficiently identify the target properties of the CAMD problem for working fluids.

In this study the CAMD problem for the development of novel working fluids for organic Rankine cycles (ORC) is formulated mathematically. It integrates both a system model for the ORC and property models including the Peng-Robinson equation of state [2], for the working fluids (enthalpy, entropy, etc.) and group contribution (GC) models for pure component property predictions including critical properties as well as environmental and safety related properties. In addition to these property models, the system consists of coupled mass and energy balances for a pump, a condenser, a turbine and an evaporator.

As regards sensitivity analysis method, a global sensitivity analysis is performed based on Morris screening to determine which change of input parameters have important effects on the net power output. The screening is composed of individually randomized one-factor-at-a-time parameter changes over the whole parameter space [3]. This allows users to identify which properties are important (as well optimal region of property values) hence can be candidate as target properties for a working fluid design and/or search. In addition, environmental and safety properties such as the ozone depletion potential (ODP), the global warming potential (GWP) as well as flammability limits are taken into account to give a multi-criteria framework.

Furthermore, a process optimization with respect to the properties is performed to identify the optimal property values for a given process set-up [4]. This in combination with the sensitivity analysis to specify systematically the boundaries for the cycle related target properties. This facilitates an efficient screening for the optimal pure components or mixture working fluids.

The methodology will be applied in a case study of an Organic Rankine Cycle (ORC) with a low-temperature heat source. The heat source is a hot water stream from waste heat of a chemical site. Giving this pre-exquisite the method allows to identify the most favorable working fluid along with the corresponding optimal process conditions in order to get the highest possible power output.

The study presents a new approach for the identification of target properties of CAMD problems based on sensitivity analysis and shows its application for the development of novel working fluids of organic Rankine cycles for low temperature heat sources.

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**Shape and topology optimization of enzymatic microreactors**

Structural optimization methods have been used by mechanical and civil engineers over the years to find the optimal structures. Structural optimization is a series of computational techniques which include shape and topology optimization. Shape optimization is directly applied to the boundaries of a structure and results in the deformation of the configuration. Topology optimization contributes to the improvement of the layout of the material in a domain. The mechanical performance of a structure is evaluated by an objective function which can be for example maximizing its stiffness. The need for effective and cost efficient reactors for pharmaceutical processes forces the industry to search for better technologies. In biochemical engineering, the used reactor design in a given process is usually limited to a range of well-established configurations and layouts. Usually the implemented reactors in a chemical process do not always yield in the best reaction conditions. This thesis develops an innovative application of topology and shape optimization methods to a chemical engineering problem. The main goal is to design a reactor according to the limitations of the reaction system by modifying the reactor configuration. In this thesis structural optimization methods were exclusively applied to enzymatic microreactors. The case studies were chosen such that they can be experimentally tested afterwards. In this way, the design of the reactor is customized to the reaction system and it contributes to the reduction of extensive experimental work to find the best reactor configuration. Shape optimization has been applied to an YY-microreactor with a rectangular cross-section with the intention to investigate the shape influence on the active mixing of substances and consequently in the reaction yield. The inlet and the outlet are located at the respective ends of the reactor. Both inlet and outlet have a Y shape where two streams meet at the entrance of the reaction chamber and two streams are split again at the exit.
The capability of membrane-active peptides to disrupt phospholipid membranes is often studied by investigating peptide-induced leakage of quenched fluorescent molecules from large unilamellar lipid vesicles. In this article, we explore two fluorescence microscopy-based single-vesicle detection methods as alternatives to the quenching-based assays for studying peptide-induced leakage from large unilamellar lipid vesicles. Specifically, we use fluorescence correlation spectroscopy (FCS) to study the leakage of fluorescent molecules of different sizes from large unilamellar lipid vesicles dispersed in aqueous solution, and we use confocal imaging of surface-immobilized large unilamellar lipid vesicles to investigate whether there are heterogeneities in leakage between individual vesicles. Of importance, we design an experimental protocol that allows us to quantitatively correlate the results of the two methods; accordingly, it can be assumed that the two methods provide complementary information about the same leakage process. We use the two methods to investigate the membrane-permeabilizing activities of three well-studied cationic membrane-active peptides: mastoparan X, melittin, and magainin 2. The FCS results show that leakage induced by magainin 2 is less dependent on the size of the encapsulated fluorescent molecules than leakage induced by mastoparan X and melittin. The confocal
imaging results show that all three peptides induce leakage by a heterogeneous process in which one portion of the vesicles are completely emptied of their contents but another portion of the vesicles are only partially emptied. These pieces of information regarding leakage induced by mastoparan X, melittin, and magainin 2 could not readily have been obtained by the established assays for studying peptide-induced leakage from lipid vesicles.

**General information**

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Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Center for Nanomedicine and Theranostics, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Chemistry, Physical and Biophysical Chemistry
Authors: Kristensen, K. (Intern), Ehrlich, N. (Intern), Henriksen, J. R. (Intern), Andresen, T. L. (Intern)
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BFI (2012): BFI-level 2
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Solubility of hydrogen sulfide in aqueous solutions of N-methyldiethanolamine at high pressures

A static-analytic method was used to measure the H2S solubility in 50 wt% MDEA and in presence of methane as a makeup gas. The solubility was measured at 7000 kPa total pressure, and at 50 and 70 degrees C, for H2S partial pressures from 31 to 974 kPa. Measurements were also performed at 1500 kPa total pressure and 50 degrees C for H2S partial pressure span of 53-386 kPa. The measured data were compared to predictions using the Extended UNIQUAC model. The experimental data showed that the total pressure has a significant effect on H2S solubility in aqueous MDEA. The observed effect is shown to be dominated by the non-ideality of the gas, and it could be predicted by the pressure effect on the fugacity coefficient of H2S in the gas phase. The experimental data from this work are compared and shown to be consistent with earlier published data.
State Estimation in Fermentation of Lignocellulosic Ethanol. Focus on the Use of pH Measurements.

The application of the continuous-discrete extended Kalman filter (CD-EKF) as a powerful tool for state estimation in biochemical systems is assessed here. Using a fermentation process for ethanol production as a case study, the CD-EKF can effectively estimate the model states even when highly non-linear measurements such as pH are included. Several configurations of the CD-EKF are tested and it is seen that including pH, which is a readily available measurement in virtually every biochemical process, provides information that significantly improves the performance of the filter.

General information
Enzymes have recently been considered as possible agents for enhanced oil recovery (EOR) acting at the liquid-solid interface. One way to assess this is via measuring the wettability of calcite surfaces, important for EOR methods in carbonaceous reservoirs. In the present work, we have experimentally investigated the effect of enzymes on the wettability of calcite mineral surfaces with oil-brine systems. The action of various enzymes, including esterases/lipases, carbohydrases, proteases and oxidoreductases (along with two commercial mixtures) was studied by contact angle measurements and adhesion behaviour tests. Comparative studies with a surfactant, protein, purified enzyme, enzyme stabiliser using n-decane (as a model for the oil) have also been carried out in order to verify experimental results. The enzymes that have the highest effect on the wettability have been identified. Those enzymes, which were found the most promising from a practical perspective, have shown the ability to fully detach oil from the surface, even at very low enzyme concentrations. For example, esterases/lipases were found to strongly affect the wettability and to remove adhesion at concentrations as low as 0.1% of the enzyme product (corresponding to 0.002-0.005% protein). Likewise, proteases could also improve wettability, although the effect was not consistent and was dependent on impurities. Other enzymes had no effect on the wettability of calcite at the concentration studied. The main mechanism of enzymatic action has been found to be replacement of oil at the solid surface by the enzyme. Other mechanisms (modification of the surface tension or catalytic modification of hydrocarbons resulting in reducing the oil viscosity) have shown to be much less pronounced from the measurements reported here.
Adhesion, Carbonaceous reservoirs, Enhanced oil recovery, Enzymes, Wettability, Calcite, Esters, Oil shale, Paraffins, Petroleum reservoir engineering, Phase interfaces, Proteins, Wetting, Catalytic modifications, Commercial mixtures, Comparative studies, Enzymatic action, Enzyme concentrations, Liquid-solid interfaces, Oxido-reductases, Enhanced recovery

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Superstructure-based optimization of biorefinery networks: Production of biodiesel

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 as biorefineries [2]. The optimal synthesis of biorefinery networks problem is defined as: given a set of biomass derived feedstock and a set of desired final products and specifications, determine a flexible, sustainable and innovative processing network with the targets of minimum cost and sustainable development taking into account the available technologies, geographical location, future technological developments and global market changes.

The problem of optimal design of biorefinery networks is solved in this work through three different stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. At the synthesis stage, the considered alternatives are represented in a
superstructure, from which a mixed-integer linear or nonlinear programming (MILP or MINLP) problem is derived and
solved in order to find the optimal processing network for a pre-defined objective function. Next, at the design stage, the
selected processing network is simulated and analyzed and targets for improvement are identified. Finally, a more
sustainable design is achieved at the innovation stage by generating innovative solutions that satisfy the targets from the
design stage.

The applicability of the proposed approach is shown through a practical case study for the production biodiesel from a
variety of feedstock. The different biorefinery processing alternatives are represented in a superstructure and the
associated data is collected and stored in a database. Once a specific biorefinery synthesis problem is formulated, the
superstructure is reduced in order to include only the relevant alternatives. The reduced superstructure is represented
using mathematical models - the modelling approach by Quaglia et al. [3] is used - and solved to find the optimal network
for different scenarios.

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Sustainable design of chemical and biochemical processes: The role of models & modelling

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Sustainable Process Design under uncertainty analysis: targeting environmental indicators

This study focuses on uncertainty analysis of environmental indicators used to support sustainable process design efforts. To this end, the Life Cycle Assessment methodology is extended with a comprehensive uncertainty analysis to propagate the uncertainties in input LCA data to the environmental indicators. The resulting uncertainties in the environmental indicators are then represented by empirical cumulative distribution function, which provides a probabilistic basis for the interpretation of the indicators. In order to highlight the main features of the extended LCA, the production of biodiesel from algae biomass is used as a case study. The results indicate there are considerable uncertainties in the calculated environmental indicators as revealed by CDFs. The underlying sources of these uncertainties are indeed the significant variation in the databases used for the LCA analysis. The extended LCA procedure is flexible and generic and can handle various sources of uncertainties in environmental impact analysis. This is expected to contribute to more reliable calculation of impact categories and robust sustainable process design.

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Sustainable process synthesis-intensification

Chemical industry is facing global challenges such as the need to find sustainable production processes. Process intensification as part of process synthesis has the potential to find truly innovative and more sustainable solutions. In this paper, a computer-aided, multi-level, multi-scale framework for synthesis, design and intensification of processes, for identifying more sustainable alternatives is presented. Within the framework, a three stage work-flow has been implemented where, in the first “synthesis” stage an optimal processing route is synthesized through a network superstructure optimization approach and related synthesis tools. In the second, “design” stage, the processing route from the first stage is further developed and a base case design is established and analyzed. In the third, “innovation” stage, more sustainable innovative solutions are determined. The application of the framework is illustrated through a case study related to the production of di-methyl carbonate, which is an important bulk chemical due to its multiplicity of uses.

General information
Synthesis and Design of a Sustainable CO2 Utilization Network

In response to increasing regulations and concern about the impact of greenhouse gases on the environment, carbon dioxide (CO2) emissions are targeted for reduction. One method 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 a case study on the methanol synthesis processing block. CO2 conversion processes show promise as an additional method for the sustainable reduction of CO2 emissions.

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Synthesis and Design of Integrated Process and Water Networks

This work presents the development of a systematic framework for a simultaneous synthesis and design of process and water networks using the superstructure-based optimization approach. In this framework, a new superstructure combining both networks is developed by attempting to consider all possible options with respect to the topology of the process and water networks, leading to Mixed Integer Non Linear Programming (MINLP) problem. A solution strategy to solve the multi-network problem accounts explicitly the interactions between the networks by selecting suitable technologies in order to transform raw materials into products and produce clean water to be reused in the process at the early stage of design. Since the connection between the process network and the wastewater treatment network is not a straight forward connection, a new converter interval is introduced in order to convert the values of contaminants in the wastewater stream into wastewater characterizations. The systematic approach is used to manage the complexity of the problem by solving simultaneously process synthesis and water synthesis network problems with respect to environment, economics and sustainability. The applicability of the systematic approach is demonstrated using a conceptual case study to test the features of the solution approach under different scenarios depending on the design-synthesis problem.

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Synthesis and design of optimal biorefinery

Chemical manufacturing, transportation fuels production and power plants among other sectors have strongly depended on fossil-based resources. To support sustained economic growth, additional fossil-based resources are required, but, inevitably, this also has a major impact on the global environment. These challenges motivate the development of sustainable technologies for processing renewable feedstock for the production of fuels, chemicals and materials in what is commonly known as a biorefinery. The biorefinery concept is a term to describe one or more processes which produce various products from bio-based feedstock. Since there are several bio-based feedstock sources, this has motivated development of different conversion concepts producing various desired products. This results in a number of challenges for the synthesis and design of the optimal biorefinery concept at the early-stage of process development: (i) Combinatorial challenge: a large number of potential processing paths resulting from the combination of many potential feedstocks, and many available conversion technologies to produce a number of desired products; (ii) Data challenge: the data typically used for early stage process feasibility analysis is of a multidisciplinary nature, often limited and uncertain; (iii) Complexity challenge: this problem is complex requiring multi-criteria evaluation (technical, economic, sustainability).

This PhD project aims to develop a decision support tool for identifying optimal biorefinery concepts at the early-stage of product-process development. To this end, a systematic framework has been developed, including a superstructure-based optimization approach, a comprehensive database of processing and conversion technologies, and model libraries to allow generation and comparison of a large number of alternatives at their optimality. The result is the identification of the optimal raw material, the product (single vs multi) portfolio and the corresponding process technology selection for a given market scenario. The economic risk of investment due to market uncertainties is further analysed to enable risk-aware decision making. The application of the developed analysis and decision support toolbox is highlighted through relevant biorefinery case studies: bioethanol, biogasoline or biodiesel production; algal biorefinery; and bioethanol-upgrading concepts are presented. This development and analysis provides a robust guidance to support the development of sustainable and future biorefineries.

Synthesis of 5-hydroxymethylfurfural (HMF) by acid catalyzed dehydration of glucose-fructose mixtures

Synthesis of 5-hydroxymethylfurfural (HMF) from hexoses has been studied extensively in the scientific literature. However, a process has yet to be implemented at industrial scale. In this paper the simultaneous dehydration of glucose...
and fructose was investigated, in order to develop a process allowing the use of the cheapest available source of fructose: high fructose corn syrup. The dehydration was catalyzed by hydrochloric acid and conducted in acetone-water mixtures, which ensured good selectivity towards HMF and eliminated precipitation of polymer by-products (insoluble humins). Through a detailed experimental investigation a reaction network was proposed, and subsequently the corresponding kinetic model was fitted to experimental data in order to obtain estimates of the reaction kinetic parameters. The kinetic model is capable of predicting the formation of HMF along with the important by-products: soluble humins, glucose dimers, anhydroglucose, and formic acid. The reaction conditions in four different reactor configurations were optimized and compared using the kinetic model. It was found that a recirculating reactor setup is preferable, where the equilibrium controlled by-products (anhydroglucose and glucose dimers) are recirculated to the dehydration reactor. The model predicts an HMF selectivity of close to 70% in a recirculating reactor at conditions where HMF degradation is avoided.

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Synthesis of biorefinery networks using a superstructure optimization based approach

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 as biorefineries [2]. The optimal synthesis of biorefinery networks problem is defined as: given a set of biomass derived feedstock and a set of desired final products and specifications, determine a flexible, sustainable and innovative processing network with the targets of minimum cost and sustainable development taking into account the available technologies, geographical location, future technological developments and global market changes. The problem of optimal design of biorefinery networks is solved in this work through three different stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. At the synthesis stage, the considered alternatives are represented in a superstructure, from which a mixed-integer linear or nonlinear programming (MILP or MINLP) problem is derived and solved in order to find the optimal processing network for a predefined objective function. Next, at the design stage, the selected processing network is simulated and analyzed and targets for improvement are identified. Finally, a more sustainable design is achieved at the innovation stage by generating innovative solutions that satisfy the targets from the design stage. This work is concerned with the first stage: the synthesis stage. Various biorefinery processing alternatives are represented in a superstructure and the superstructure is reduced in order to include only the relevant alternatives. The superstructure is reduced based on constraints from the problem formulation, such as location or raw material. The reduced superstructure is then represented using mathematical models - the modelling approach by Quaglia et al. [3] is used - and solved to find the optimal network. The applicability of the proposed approach is shown through a practical case study for the production of valuable products (i.e. lysine and lactic acid) from sugarcane molasses; these alternatives are considered with respect to availability and demands in Mexico [4].

Synthesis of Optimal Processing Pathway for Microalgae-based Biorefinery under Uncertainty

The research in the field of microalgae-based biofuels and chemicals is in early phase of the development, and therefore a wide range of uncertainties exist due to inconsistencies among and shortage of technical information. In order to handle and address these uncertainties to ensure robust decision making, we propose a systematic framework for the synthesis and optimal design of microalgae-based processing network under uncertainty. By incorporating major uncertainties into the biorefinery superstructure model we developed previously, a stochastic mixed integer nonlinear programming (sMINLP) problem is formulated for determining the optimal biorefinery structure under given parameter uncertainties modelled as sampled scenarios. The solution to the sMINLP problem determines the optimal decisions with respect to processing technologies, material flows, and product portfolio in the presence of uncertain parameters. The developed framework is implemented and tested on a specific case study, to identify the promising processing pathway for the production of biofuels from microalgae while accounting for modelled uncertainties.
Systematic Computer-Aided Framework for Sustainable Chemical Product Design

Computer-aided product design (CAPD) is a method for the generation and selection of novel pure, mixed and blended chemical products [1]. In CAPD, the chemical product is generated and selected based on defined structure, property and process/application constraints. Several challenges exist for CAPD, including the accuracy of the property estimation, molecular structure generation, inclusion of sustainability, process and application targets and needs in the problem formulation. CAPD has been widely utilized for the synthesis of several types of products, such as solvents, polymers, fuels and formulated products [2]. However, for product design problems where the process needs and sustainability possess demanding constraints, the complexity of the problem is increased as the relation between product property, sustainability and process criteria is difficult to mathematically define. In this work, a generic computer-aided framework for chemical product design is presented through a systematic framework. A CAPD problem for the generation of novel pure, mixed and blended chemical products is formulated and solved through the application of four sequential steps. In step (1), the product design problem is defined together with the process and/or application boundaries. In step (2), the CAPD problem is formulated through property constraints for pure, mixed and blended products, process/application constraints and objective function. The property constraints are carefully selected for the thermo-physical property needs and the process/application needs. Process/application and property needs are connected through an analysis of the property influence on the process/application models and thermodynamic relations. The sustainability is considered through product and process/application performance, economics and environmental impact. In step (3), the CAPD formulation is converted into a mixed-integer nonlinear program (MINLP) by set-up of constraints, objective and boundaries defined in step (2). In step (4), the MINLP is solved through a decomposed approach [3]. The decomposed approach breaks down the MINLP problem into a sub-set of programs to manage the complexity: mixed-integer linear program (MILP) for molecular generation, linear program (LP) for property constraints, non-linear program (NLP) for mixture/blend property constraints, and NLP for process constraints and objective function. This approach ensures that the optimal chemical product can be found through systematic generation and screening of alternatives based on the problem definition. The framework is implemented into a GAMS-based tool. The application of the framework is demonstrated through sustainable working fluid design for a heat pump cycle. Working fluids used in heat pumps are continuously regulated due to the environmental issues, such as ozone depletion or global warming potential. Many of the currently used working fluids are soon to be phased out [4]. The design of novel working fluids is a challenging task as retro-fitting as well as re-designing demand increased sustainability and minimal trade-off with system performance. In the CAPD formulation, the product properties are related to the needs of heat pump cycle and its components through sensitivity analysis of the thermodynamic models and energy balances of the system. Furthermore, simple models are included for efficient assessment of the sustainability and design criteria of both the cycle and its components. It will be demonstrated that the working fluid product designed is optimal with respect to the sustainability and the heat pump cycle performance.
Systematic Methods and Tools for Computer Aided Modelling
Models are playing important roles in design and analysis of chemicals/bio-chemicals based products and the processes that manufacture them. Model-based methods and tools have the potential to decrease the number of experiments, which can be expensive and time consuming, and point to candidates, where the experimental effort could be focused.
In this project a general modelling framework for systematic model building through modelling templates, which supports the reuse of existing models via its new model import and export capabilities, have been developed. The new feature for model transfer has been developed by establishing a connection with an external modelling environment for code generation.
The main contribution of this thesis is a creation of modelling templates and their connection with other modelling tools within a modelling framework. The goal was to create a user-friendly system, which will make the model development process easier and faster and provide the way for unified and consistent model documentation. The modeller can use the template for their specific problem or to extend and/or adopt a model. This is based on the idea of model reuse, which emphasizes the use of a model not only for one specific application but also for future applications involving different needs and levels of detail to match different purposes. As the result the model developer can generate and test models systematically, efficiently and reliably. In this way, development of products and processes can be faster, cheaper and very efficient.
The developed modelling framework involves five main elements: 1) a modelling tool, that includes algorithms for model generation; 2) a template library, which provides building blocks for the templates (generic models previously developed); 3) computer aided methods and tools, that include procedures to perform model translation, model analysis, model verification/validation, model solution and model documentation; 4) model transfer – export/import to/from other application for further extension and application – several types of formats, such as XML-format and COM-objects, are incorporated to allow the export and import of mathematical models; 5) a user interface that provides the work-flow and data-flow to guide the user through the different modelling tasks.

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System-wide Benchmark Simulation Model for integrated analysis of urban wastewater systems

Interactions between different components (sewer, wastewater treatment plant (WWTP) and river) of an urban wastewater system (UWS) are widely recognized (Benedetti et al., 2013). This has resulted in an increasing interest in the modelling of the UWS. System-wide models take into account the interactions between the different subsystems and allow us to operate the UWS in a holistic manner. Such an integrated approach makes it feasible to evaluate control strategies at an UWS scale with the aim of improving receiving water quality.

Currently, benchmark simulation models are widely used to evaluate local and plant-wise control strategies in WWTPs (Jeppsson et al., 2013). The International Water Association (IWA) Benchmark Simulation Models (BSM1, BSM1_LT, BSM2) consist of a predefined plant layout, process models, sensor and actuator models, influent characteristics and evaluation criteria (Gernaey et al., 2014). Given the success of BSMs in evaluation of control strategies for WWTPs, it is envisioned to spatially expand the plant-wide BSM to a system-wide tool. A system-wide BSM can then play an important role, not only in the evaluation of integrated control strategies, but also in developing a better understanding of the interactions between different components of an UWS.

This paper aims at presenting a system-wide benchmark simulation model that includes catchment, sewer network, WWTP and receiving water subsystems. A hypothetical UWS layout is defined and an integrated model for this system is developed. Modelling details for various building blocks of the model are explained in the following sections of this abstract. Preliminary simulation results are used to evaluate the impact of rain events using indirect (emission measures from sewers and WWTPs) and direct (river quality based) measures. We demonstrate the need of using a holistic approach due to the strong interactions between the elements of the UWS (catchment, WWTP and sewer).

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Techno-economic evaluation of different CO2-based processes for dimethyl carbonate production

In this work, several chemical processes for production of dimethyl carbonate (DMC) based on CO2 utilization are evaluated. Four CO2-based processes for production of DMC are considered: (1) direct synthesis from CO2 and methanol; (2) synthesis from urea; (3) synthesis from propylene carbonate; and (4) synthesis from ethylene carbonate. The processes avoid the use of toxic chemicals such as phosgene, CO and NO that are required in conventional DMC production processes. From preliminary thermodynamic analysis, the yields of DMC are found to have the following order (higher to lower): ethylene carbonate route > urea route > propylene carbonate route > direct synthesis from CO2. Therefore, only the urea and ethylene carbonate routes are further investigated by comparing their performances with the commercial BAYER process on the basis of kg of DMC produced at a specific purity. The ethylene carbonate route is found to give the best performance in terms of energy consumption (11.4% improvement), net CO2 emission (13.4% improvement), in global warming potential (58.6% improvement) and in human toxicity-carcinogenic (99.9% improvement) compared to the BAYER process. Also, the ethylene carbonate option produces ethylene glycol as a valuable by-product. Based on the above and other performance criteria, the ethylene carbonate route is found to be a highly promising green process for DMC production. © 2014 The Institution of Chemical Engineers.
Techno-economic risk analysis of glycerol biorefinery concepts against market price fluctuation

A biorefinery integrates biomass conversion processes to produce fuels, power, and chemicals from bio-based feedstock. Through the synthesis of several products, a biorefinery can benefit from the differences in biomass composition and make the most of the value derived from the biomass feedstock. The high-value added bio-products boost profitability, the high-volume fuel helps meet national energy targets, and the power production cuts costs and dodges greenhouse-gas emissions [1] [2] [3]. The increasing amount of biodiesel production worldwide (e.g. from vegetable oils, palm oil, animal fats or recycled greases as feedstock) is generating a large amount of waste crude glycerol as a by-product (for every 10 kg of biodiesel, 1 kg of waste glycerol is produced) [4]. This worldwide increase in biodiesel production led to a surplus in glycerol which subsequently leads to a decrease in the crude glycerol prices. Therefore, in order to increase the economic competitiveness of the biodiesel industry, there is an increasing interest in adding value using the glycerol waste stream as feedstock for the synthesis of bio-derived building block compounds and polymers [5] [6] [7] [8] [4] [9]. Moreover, certain algae species also accumulate large amounts of glycerol and could become another possible source due to the recent development of algae biomass as feedstock for biofuel production [10]. In this contribution, we study and critically analyze a number of glycerol biorefinery concepts developed earlier [11][12][13][14][15] and compare them in terms of techno-economic performance including minimum selling price calculation for potential high-value added products. In particular, we address the challenge of price volatility (both glycerol as feedstock and high-value added chemicals) and the associated economic risks against historical market fluctuations when assessing the economics of competing glycerol biorefinery concepts. The aim is to compare the fitness/survival of the biorefinery concepts under extreme market disturbances. To perform this analysis, we used a superstructure based sustainable design framework developed earlier [16] [1] [17] [10]. The economic risk analysis enables the user to perform a comprehensive assessment of alternatives using a probabilistic framework which helps to design a robust and competitive glycerol biorefinery.
The coupling of ω-transaminase and Oppenauer oxidation reactions via intra-membrane multicomponent diffusion – A process model for the synthesis of chiral amines

In this study we consider the theoretical coupling of an otherwise thermodynamically limited ω-transaminase reaction to an Oppenauer oxidation, in order to shift the equilibria of both reactions, with the aim of achieving a significant (and important) increase in the yield of the desired chiral amine product. Using 2-propylamine as the amine donor of the ω-transaminase reaction, gives acetone as a by-product, which in turn allows the coupling of the ω-transaminase reaction with the Oppenauer oxidation. The Oppenauer reaction converts secondary alcohols into ketones, and these can subsequently be fed to the ω-transaminase reaction. In this way, one of the products of the ω-transaminase reaction becomes the reactant of the Oppenauer reaction, and vice versa, creating a cycle which shifts the equilibria of both reactions. Such coupled reactions are frequently found in nature. The purpose of this paper is to report the development of a mathematical model as a tool for the simulation and potential design of such a process for the production of a range of chiral amines. The mathematical model developed considers that each reaction is performed in a single ideally mixed isothermal reactor operating sequentially in fed batch–batch mode. Both reactors are interconnected through a semi-permeable membrane, where multicomponent intra-membrane transport takes place by diffusion and viscous flow. The kinetic modeling of both reactions has been carried out and model simulations show that in this way a significant increase in the yield of the chiral amine product may be obtained. Finally, the role of the different parameters involved in the process model has been analyzed.
Thermodynamic Calculations for Systems Biocatalysis

'Systems Biocatalysis' is a term describing multi-enzyme processes in vitro for the synthesis of chemical products. Unlike in-vivo systems, such an artificial metabolism can be controlled in a highly efficient way in order to achieve a sufficiently favourable conversion for a given target product on the basis of kinetics. However, many of the most interesting non-natural chemical reactions which could potentially be catalysed by enzymes, are thermodynamically unfavourable and are thus limited by the equilibrium position of the reaction. A good example is the enzyme ω-transaminase, which catalyses the transamination of a pro-chiral ketone into a chiral amine (interesting in many pharmaceutical applications). Here, the products are often less energetically stable than the reactants, meaning that the reaction may be thermodynamically unfavourable. As in nature, such thermodynamically-challenged reactions can be altered by coupling with other reactions. For instance, in the case of ω-transaminase, such a coupling could be with alanine dehydrogenase. Herein, the aim of this work is to identify thermodynamic bottlenecks within a multi-enzyme process, using group contribution method to calculate the Gibbs free energy change, $\Delta G^0_r$, of the overall cascade. The findings show that unfavourable reactions in the cascade can be improved by coupling to a favourable reaction giving more energetically stable products.

General information

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Abu, R. (Intern), Gundersen, M. T. (Intern), Woodley, J. M. (Intern)
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Systems Biocatalysis, Multi-enzyme, Thermodynamics, Group contribution
Thermodynamic modeling of hydrogen sulfide absorption by aqueous N-methyldiethanolamine using the Extended UNIQUAC model

Aqueous MDEA is the most commonly used solvent for H2S removal from natural gas. A reliable thermodynamic model is required for the proper design of natural gas sweetening processes. In this study, a rigorous thermodynamic model is developed to represent properties of the H2S-MDEA-H2O ternary system. The Extended UNIQUAC model is used to represent the system behavior. The model is created based on models for the constituent binary subsystems. The developed model provides accurate representation of VLE and heat of absorption for the studied system and subsystem in the temperature range of 0-180°C, H2S partial pressure of 0.0033-8329.71kPa, MDEA mass% of 0-50 and loading range of 0-2.17.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering
Authors: Sadegh, N. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
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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
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Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
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Scopus rating (2009): SJR 1.133 SNIP 1.164
Thermodynamic Modeling of Multi-phase Solid–Liquid Equilibria in Industrial-Grade Oils and Fats

Compositional thermodynamic phase separation is investigated for industrial-grade vegetable oils with complex compositions. Solid–liquid equilibria have been calculated by utilizing the Margules 2-suffix activity-coefficient model in combination with minimization of the Gibb’s free energy of the system. On the basis of quasi-equilibrium solid-fat content (SFC) measurements, a new approach to the estimation of the interaction parameters, needed for the activity-coefficient model, has been developed. The parameters are fitted by matching the SFC of two oils at various degrees of dilution and isothermal temperatures. Subsequently, the parameters are successfully validated against three oils, rich in asymmetric and symmetric triacylglycerols (TAG), respectively. The new approach developed is shown to be very flexible, allowing incorporation of additional TAG and polymorphic states. It thereby provides a simple way to dealing with multi-component, multi-phase TAG mixtures without having the required binary interaction parameters at hand a priori. This ultimately provides a powerful, predictive tool which may serve as a starting point for laboratory screening and creation of tailor-made products because many different oil mixtures can be evaluated quickly with respect to specific properties, prior to more time-consuming experimental evaluation.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CHEC Research Centre, Aak Denmark A/S
Authors: Hjorth, J. L. (Ekstern), Miller, R. L. (Ekstern), Woodley, J. M. (Intern), Kiil, S. (Intern)
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Topology optimization for biocatalytic microreactor configurations
The aim of this study is to present an innovative strategy for selecting a reactor for a specific process. Instead of adapting the process to a well-known reactor shape, a topology optimization method is used to obtain the best reactor configuration, and is applied to a biocatalytic reaction system as a case study. The Evolutionary Structure Optimization (ESO) method is applied using an interface between Matlab® and the computational fluid dynamic simulation software ANSYS CFX®. In the case study, the ESO method is applied to optimize the spatial distribution of immobilized enzyme inside a microreactor. The results allow evaluating which regions in the microreactor have more importance for the product formation. In fact, it was possible to simulate the improvement of the outlet product concentration per same amount of enzyme by modifying the spatial distribution of the immobilized enzyme.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Pereira Rosinha, I. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Krühne, U. (Intern)
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Uncertainties in early-stage capital cost estimation of process design – a case study on biorefinery design
Capital investment, next to the product demand, sales, and production costs, is one of the key metrics commonly used for project evaluation and feasibility assessment. Estimating the investment costs of a new product/process alternative during early-stage design is a challenging task, which is especially relevant in biorefinery research where information about new technologies and experience with new technologies is limited. A systematic methodology for uncertainty analysis of cost data is proposed that employs: (a) bootstrapping as a regression method when cost data are available; and, (b) the Monte Carlo technique as an error propagation method based on expert input when cost data are not available. Four well-known models for early-stage cost estimation are reviewed and analyzed using the methodology. The significance of uncertainties of cost data for early-stage process design is highlighted using the synthesis and design of a biorefinery as a case study. The impact of uncertainties in cost estimation on the identification of optimal processing paths is indeed found to be profound. To tackle this challenge, a comprehensive techno-economic risk analysis framework is presented to enable robust decision-making under uncertainties. One of the results using order-of-magnitude estimates shows that the production of diethyl ether and 1,3-butadiene are the most promising with the lowest economic risks (among the alternatives considered) of 0.24 MM$/a and 4.6 MM$/a, respectively.

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Authors: Cheali, P. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
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Volume: 3
Article number: 3
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In this study, several strategies to upgrade lignocellulosic biorefineries for production of value-added chemicals are systematically generated and evaluated with respect to economic and sustainability objectives. A superstructure-based process synthesis approach under uncertainty integrated with a sustainability assessment method is used as evaluation tool. First, an existing superstructure representing the lignocellulosic biorefinery design network is extended to include the options for catalytic conversion of bioethanol to value-added derivatives. Second, the optimization problem for process upgrade is formulated and solved for two different objective functions: i) maximization of operating profit (the techno-economic criterion); and ii) minimization of the sustainability single index ratio (the sustainability criterion). These results indicate first that there is a significant potential of improvement of operating profit for biorefineries producing bioethanol-derived chemicals (247 MM$/a and 241 MM$/a for diethyl ether and 1,3-butadiene, respectively). Second, the optimal designs for upgrading bioethanol (i.e. production of 1,3-butadiene and diethyl ether) performed also better with respect to sustainability compared with the petroleum-based processes. In both cases, the effects of the market price uncertainties were also analyzed by performing quantitative economic risk analysis and presented a significant risk of investment for a lignocellulosic biorefinery (12 MM$/a and 92 MM$/a for diethyl ether and 1,3-butadiene, respectively). The multi-product biorefinery presented a more robust and risk-aware upgrading strategy considering the uncertainties that are typical for a long-term investment horizon.
Upgrading the Benchmark Simulation Model Framework with emerging challenges - A study of N₂O emissions and the fate of pharmaceuticals in urban wastewater systems

Nowadays a wastewater treatment plant (WWTP) is not only expected to remove traditional pollutants from the wastewater; other emerging challenges have arisen as well. A WWTP is now, among other things, expected to also minimise its carbon footprint and deal with micropollutants. Optimising the performance of a WWTP can be done with mathematical models that can be used in simulation studies. The Benchmark Simulation Model (BSM) framework was developed to compare objectively different operational/control strategies. As different operational strategies of a WWTP will most likely have an effect on the greenhouse gas (GHG) emissions and the removal rate of micropollutants (MPs), modelling these processes for dynamic simulations and evaluation seems to be a promising tool for optimisation of a WWTP. Therefore, in this thesis the BSM is upgraded with processes describing GHG emissions and MPs removal. Regarding GHGs emissions, the focus is placed on the production of nitrous oxide (N₂O). As micropollutants comprise a wide range of chemicals, pharmaceuticals are selected here as specific examples to be studied. Different nitrification
models containing N2O producing processes are tested and used for an extension of the BSM. Various challenges were encountered regarding the mathematical structure and the parameter values when expanding the BSM. The N2O models produced different results due to the assumptions on which they are based. In addition, pH and inorganic carbon concentrations have been demonstrated to significantly influence the nitrification. Therefore a physicochemical model in combination with a N2O model is calibrated with data from a full-scale sequencing batch reactor (SBR) to gain insight into the N2O production pathways. Most likely the pathways of nitrifier denitrification and hydroxylamine oxidation alternated during the nitrification phase in the SBR. The BSM framework is also extended with the occurrence, transport and fate of pharmaceuticals. The occurrence is modelled with a phenomenological approach for pharmaceuticals, including a daily pattern and a stochastic approach for pharmaceuticals with a more random occurrence. Different sewer conditions demonstrated effects on the occurrence of the pharmaceuticals as influent patterns at the inlet of the WWTP were smoothed or delayed. The fate in the WWTP showed that operational conditions can influence the biotransformation, retransformation and sorption rates. In addition, inhibition and co-metabolic effects can have opposite effects on the removal rates. A phenomenological influent generator has been successfully calibrated with high frequency data for traditional variables and data on the occurrence of pharmaceuticals and metabolites. The excretion pathways as well as in-sewer transformation processes proved to be of importance when calibrating the daily patterns. Upgrading the BSM framework with these calibrated models can help to optimise the performance of a WWTP by not only taking operational costs and effluent quality into account, but also by including the GHG emissions and removal rates of pharmaceuticals.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering, Urban Water Engineering
Authors: Snip, L. (Intern), Plósz, B. G. (Intern), Flores Alsina, X. (Intern), Jeppsson, U. A. C. (Ekstern), Gernaey, K. (Intern)
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Use of operating windows for assessment of continuous plug flow slurry reactor

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, AstraZeneca
Authors: Singh, R. (Intern), Gregertsen, B. (Ekstern), Muller, F. (Ekstern), Gernaey, K. (Ekstern), Gani, R. (Intern), Woodley, J. (Intern)
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Validation of a functional model for integration of safety into process system design

Qualitative modeling paradigm offers process systems engineering a potential for developing effective tools for handling issues related to Process Safety. A qualitative functional modeling environment can accommodate different levels of abstraction for capturing knowledge associated with the process system functionalities as required for the intended safety applications. To provide the scientific rigor and facilitate the acceptance of qualitative modelling, this contribution focuses on developing a scientifically based validation method for functional models. The Multilevel Flow Modeling (MFM) methodology is adopted in the paper as a formalized qualitative functional modeling methodology for dynamic process
systems. A functional model validation procedure is proposed to assess whether the intended modeling purpose indeed represents a relevant proposal and whether the model represents the system behavior sufficiently well. With the reasoning capability provided by the MFM syntax and semantics, the validation procedure is illustrated on a three-phase separator system of an MFM model. The MFM model reasoning results successfully compares against analysis results from API RP 14-C.

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Organisations: Department of Chemical and Biochemical Engineering, Department of Electrical Engineering, Automation and Control, Center for Electric Power and Energy, Energy system operation and management. CAPEC-PROCESS
Authors: Wu, J. (Intern), Lind, M. (Intern), Zhang, X. (Intern), Jørgensen, S. B. (Intern), Sin, G. (Intern)
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**Vapour liquid equilibria of monocaprylin plus palmitic acid or methyl stearate at \( P = (1.20 \text{ and } 2.50) \text{ kPa} \) by using DSC technique**

The Differential Scanning Calorimetry (DSC) technique is used for measuring isobaric (vapour+liquid) equilibria for two binary mixtures: \{monocaprylin+palmitic acid (system 1) or methyl stearate (system 2)\} at two different pressures \( P = (1.20 \text{ and } 2.50) \text{ kPa} \). The obtained PTx data are correlated by Wilson, NRTL and UNIQUAC models. The original UNIFAC group contribution method is also considered and new binary interaction parameters for the main groups CH2, CCOO, OH and COOH are regressed, to account for the non-idealities found in these lipid systems. Established thermodynamic consistency tests are applied and attest the quality of the measured data. In terms of relevance of the selected components, system 1 can be found in the purification and deodorization steps during the production of edible oils, while, system 2 can be found in the purification steps of biodiesel. It should be noted that no such data could be found in the open literature, not only for the specific components selected but also for the combination of the classes of components considered; that is, acylglycerol plus fatty acid or fatty ester.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, State University of Campinas, Universidade Federal de Sao Paulo, Alfa Laval Copenhagen A/S
Authors: Cunico, L. P. (Intern), Damaceno, D. S. (Ekstern), Matricarde Falleiro, R. M. (Ekstern), Sarup, B. (Ekstern), Abildskov, J. (Intern), Ceriani, R. (Ekstern), Gani, R. (Intern)
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Scopus rating (2015): SJR 1.075 SNIP 1.091 CiteScore 2.29
In this paper, the development of a systematic model-based framework for product design, implemented in the new product design software called VPPD-Lab is presented. This framework employs its in-house knowledge-based system to design and evaluate chemical products. The built-in libraries of product performance models and product-chemical property models are used to evaluate different classes of product. The product classes are single molecular structure chemicals (lipids, solvents, aroma, etc.), blended products (gasoline, jet-fuels, lubricants, etc.), and emulsified product (hand wash, detergent, etc.). It has interface to identify workflow/data-flow for the inter-related activities between knowledge-based system and model-based calculation procedures to systematically, efficiently and robustly solve various types of product design-analysis problems. The application of the software is highlighted for the case study of tailor made design of jet-fuels. VPPD-Lab works in the same way as a typical process simulator. It enhances the future development of chemical product design.
Achieving More Sustainable Designs through a Process Synthesis-Intensification Framework

More sustainable process designs refer to design alternatives that correspond to lower values of a set of targeted performance criteria. In this paper, a multi-level framework for process synthesis-intensification that leads to more sustainable process designs is presented. At the highest level of aggregation, process flowsheets are synthesized in terms of a sequence of unit operations that correspond to acceptable values for a set of targeted performance criteria. This defines the upper-bound of the performance criteria and the design is called the base-case design. At the next lower level, tasks representing unit operations are identified and analyzed in terms of means-ends to find more flowsheet alternatives that improve the base-case design and correspond to lower values of the set of targeted performance criteria. At the lowest level, phenomena employed to perform the specific tasks are identified and manipulated to find intensified operations, leading to more flowsheets that further improve the base-case design and correspond to even lower values of the set of target performance criteria. An overview of the framework is presented together with a case study that highlights the key concepts and application work-flow.
A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design

The manufacture of emulsified products is of increasing interest in the consumer oriented chemical industry. Several cosmetic, household and pharmaceutical products are in the emulsified form when sold and/or they are expected to form an emulsion when used. Therefore, there is a need for the development of a methodology and relevant tools in order to spare time and resources in the design of emulsion-based chemical products, so that the products can reach the market faster and at a reduced cost. The understanding and modeling of the characteristic behavior of emulsions and their peculiar ingredients is consequently necessary to tackle this problem with computer-aided methods and tools. A comprehensive framework for the selection and design of surfactants, the main responsible for the formation and the stability of emulsions, is presented here together with the modeling of the cloud point, a key property of nonionic surfactants, with a group-contribution model. The mathematical formulation of a standard product design problem is presented, together with the list of both the pure component properties (related to nonionic surfactants) and the mixture properties (relevant to the overall products as an emulsion) needed for the solution of the design algorithm. These models are then applied together with established predictive models for pure component properties of ionic surfactants and for standard mixture properties such as the density, the viscosity, the surface and the interfacial tension, but also the type of emulsion expected (through the hydrophilic–lipophilic balance), and its stability (through the hydrophilic–lipophilic deviation), forming a robust chemical product design tool. The application of this framework is highlighted for the design of some emulsion-based chemical products.
A computer-aided framework for development, identification and management of physiologically-based pharmacokinetic models

The objective of this work is the development of a generic computer-aided modelling framework to support the development of physiologically-based pharmacokinetic models thereby increasing the efficiency and quality of the modelling process. In particular, the framework systematizes the modelling process by identifying the workflow involved and providing the required methods and tools for model documentation, construction, analysis, identification and discrimination. The application and benefits of the developed framework are demonstrated by a case study related to the whole-body physiologically-based pharmacokinetic modelling of the distribution of the drug cyclosporin A in rats and humans. Four alternative candidate models for rats are derived and discriminated based on experimental data. The model candidate that is best represented by the experimental data is scaled-up to a human being applying physiologically-based scaling laws and identifying model parameters that can be re-fitted by the limited experimental data accessible for humans using sensitivity and identifiability analysis techniques.

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Authors: Heitzig, M. (Intern), Linninger, A. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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A Dynamic Model for Cellulosic Biomass Hydrolysis: a Comprehensive Analysis and Validation of Hydrolysis and Product Inhibition Mechanisms

The objective of this study is to perform a comprehensive enzyme kinetics analysis in view of validating and consolidating a semimechanistic kinetic model consisting of homogeneous and heterogeneous reactions for enzymatic hydrolysis of lignocellulosic biomass proposed by the U.S. National Renewable Energy Laboratory (Kadam et al., Biotechnol Prog 20(3):698–705, 2004) and its variations proposed in this work. A number of dedicated experiments were carried out under a range of initial conditions (Avicel® versus pretreated barley straw as substrate, different enzyme loadings and different product inhibitors such as glucose, cellobiose and xylose) to test the hydrolysis and product inhibition mechanisms of the model. A nonlinear least squares method was used to identify the model and estimate kinetic parameters based on the experimental data. The suitable mathematical model for industrial application was selected among the proposed models based on statistical information (weighted sum of square errors). The analysis showed that transglycosylation plays a key role at high glucose levels. It also showed that the values of parameters depend on the selected experimental data used for parameter estimation. Therefore, the parameter values are not universal and should be used with caution. The model proposed by Kadam et al. (Biotechnol Prog 20(3):698–705, 2004) failed to predict the hydrolysis phenomena at high glucose levels, but when combined with transglycosylation reaction(s), the prediction of cellulose hydrolysis behaviour over a broad range of substrate concentrations (50–150 g/L) and enzyme loadings (15.8–31.6 and 1–5.9 mg protein/g cellulose for Celluclast and Novozyme 188, respectively) was possible. This is the first study introducing transglycosylation.
into the semimechanistic model. As long as these type of models are used within the boundary of their validity (substrate type, enzyme source and substrate concentration), they can support process design and technology improvement efforts at pilot and full-scale studies.

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Authors: Tsai, C. T. (Intern), Morales Rodriguez, R. (Intern), Sin, G. (Intern), Meyer, A. S. (Intern)
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Scopus rating (2016): CiteScore 1.81 SJR 0.559 SNIP 0.738
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.57 SNIP 0.74 CiteScore 1.67
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.642 SNIP 0.939 CiteScore 1.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.744 SNIP 1.024 CiteScore 2.18
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.797 SNIP 1.034 CiteScore 2.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.8 SNIP 0.947 CiteScore 1.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.7 SNIP 0.905
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 0.644 SNIP 0.715
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.52 SNIP 0.629
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.505 SNIP 0.66
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.542 SNIP 0.819
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.435 SNIP 0.692
A Framework for the Modelling of Biphasic Reacting Systems

Biphasic reacting systems have a broad application range from organic reactions in pharmaceutical and agro-bio industries to CO₂ capture. However, mathematical modelling of biphasic reacting systems is a formidable challenge due to many phenomena underlying the process such as chemical equilibrium, biphasic equilibrium, reaction kinetics, and transport/mixing. In this study, a framework for modelling biphasic reacting systems is proposed to facilitate the model development in support of model-based process design-analysis. This framework is successfully applied to describe two biphasic reaction systems: a PTC-based reaction system and pseudo-PTC system.
Alternative route of process modification for biofuel production by embedding the Fischer-Tropsch plant in existing stand-alone power plant (10 MW) based on biomass gasification - Part I: A conceptual modeling and simulation approach (a case study in Thailand)

The utilization of syngas shows a highly potential to improve the economic potential of the stand-alone power unit-based gasification plants as well as enhancing the growing demand of transportation fuels. The thermochemical conversion of biomass via gasification to heat and power generations from the earlier study is further enhanced by integrating Fischer-Tropsch (FT) synthesis with the existing gasification pilot scale studied previously. To support the potential and perspectives in major economies due to scaling up in developing countries such as Thailand, the objective of this work is to develop a base case process model coupled with techno-economic evaluation for the FT synthesis. In particular, the FT process configurations are designed and assessed using current kinetic laboratory data by our research group for modeling specific reactions in PFR reactor. The calculation of equipment sizing incurred several major unit operations is performed for once-through mode (no recycles of unconverted syngas) with electricity co-production. This study provides a detailed base-case model for the synthesis with the capacities of 1, 2 and 3 MW of syngas technology sharing and the comparison between the integrated- and non-integrated FT syntheses with respect to techno-economic criteria. The integration of FT synthesis with biomass gasification in this study results in the significant assessment of energy efficiency and cost reduction by 36.92% and 16%, respectively. (C) 2014 Elsevier Ltd. All rights reserved.
A model to assess the feasibility of shifting reaction equilibrium by acetone removal in the transamination of ketones using 2-propylamine

Acetone removal by evaporation has been proposed as a simple and cheap way to shift the equilibrium in the biocatalytic asymmetric synthesis of optically pure chiral amines, when 2-propylamine is used as the amine donor. However, dependent on the system properties, this may or may not be a suitable strategy. To avoid excessive laboratory work a model was used to assess the process feasibility. The results from the current study show that a simple model of the acetone removal dependence on temperature and sparging gas flowrate can be developed and fits the experimental data well. The model for acetone removal was then coupled to a simple model for biocatalyst kinetics and also for loss of substrate ketone by evaporation. The three models were used to simulate the effects of varying the critical process parameters and reaction equilibrium constants (K<sub>eq</sub>) as well as different substrate ketone volatilities (Henry's constant). The simulations were used to estimate the substrate losses and also the maximum yield that could be expected. The approach was seen to give a clear indication for which target amines the acetone evaporation strategy would be feasible and for which amines it would not. The study also shows the value of a modeling approach in conceptual process design prior to entering a biocatalyst screening or engineering program to assess the feasibility of a particular process strategy for a given target product. Biotechnol. Bioeng. 2014;111: 309–319. © 2013 Wiley Periodicals, Inc.
Transaminase, Biocatalysis, Acetone removal, Sparging

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Analysing drying unit performance in a continuous pharmaceutical manufacturing line by means of mass – Energy balances

The current trend in the pharmaceutical industry to move from batch-wise to continuous production processes strengthens the need for monitoring and controlling the process in-line. The ConsiGma™ continuous tableting line collects data of the different subunits in real-time, but these are not really used. In this paper the data of the six-segmented fluidized bed dryer in the line are used for the development and evaluation of a mass and energy balance. The objectives are multiple: (1) prediction of the moisture content of the granules leaving the dryer solely based on the currently logged data and (2) prediction of the gas outlet temperature to check the mass balances. Once a validated system is established the gas temperature in different horizontal sections of the drying unit can be predicted. Calculations are also used to identify errors in the system and to propose alternative sensor locations. A calibration is performed in order to predict the evaporation rate. The balances were able to predict both the moisture content of the granules at the end of the drying process and the gas outlet temperature quite accurately. Combining the gathered information with the height of the bed in the fluidized bed can be used to predict the gas temperature in different horizontal sections of the dryer. An extra sensor measuring the gas temperature and the humidity at the wet transfer line would increase the accuracy of the calculations. An extra gas velocity sensor at the outlet would be useful to incorporate an extra supervision of the calculations.

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General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Ghent University
Authors: Mortier, S. T. F. (Ekstern), Gernaey, K. (Intern), De Beer, T. D. B. (Ekstern)
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Web of Science (2013): Indexed yes
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A new paradigm for chemical engineering?

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern)
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An integrated approach for synthesis and design of process and water/wastewater networks

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Handani, Z. B. (Intern), Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2014
Event: Abstract from 21st International Congress of Chemical and Process Engineering, Prague, Czech Republic.
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

An Integrated Methodology for Emulsified Formulated Product Design
The consumer oriented chemical based products are used every day by millions of people. They are structured products constituted of numerous chemicals, and many of them, especially household and personal care products, are emulsions where active ingredients, solvents, additives and surfactants are mixed together to determine the desired emulsified product. They are still mainly designed and analysed through trial - and - error based exper- imental techniques, therefore a systematic approach , integrating model-based as well a s experiment - based techniques, for design of these products could significantly reduce both time and cost connected to product development by doing only the necessary experi- ments , and ensuring chances for innovation . The main contribution of this project i s the development of an integrated methodology for the design of emulsified formulated products. The methodology consists of three stages: the problem definition stage, the model - based design stage, and the experiment - based verification stage. In the probl em definition stage, the consumer needs are trans- lated into a set of target thermo - physical properties and into a list of categories of ingre- dients that are to be included in the formulation. In the model - based design stage, struc- tured databases, dedicated algorithms and a property model library are employed for de- signing a candidate base case formulation. Finally,
in the experiment-based verification stage, the properties and performances of the proposed formulation are measured by means of tailor-made experiments. The formulation is then validated or, if necessary, refined thanks to a systematic list of action. The problem definition stage relies on a robust knowledge base, which needs to systematically generate quantitative, useful input information for the model-based stage, starting from the consumer assessments. In the model-based stage, comprehensive chemical databases, consistent property models and a dedicated algorithm for the design of emulsified solvent mixtures are needed. Finally, for the experiment-based stage, an efficient planning of the experiments is required, together with the systematic generation of a list of actions to be taken; in case some of the experiments do not validate the candidate formulation generated in the previous stage. All the above mentioned issues are addressed in this PhD work: the necessary property models have been retrieved and organized in a model library; new property models have been developed for a set of thermo-physical properties of surfactants; a robust, systematic knowledge-base has been developed in relation to emulsified formulated products; chemical databases have been improved and generated; and an algorithm for the model-based design of emulsified solvent mixtures has been developed. All these tools have been implemented as a new template in the virtual Product-Process Design laboratory software. To illustrate the application of the proposed methodology, three case studies have been developed. For one of these case studies, the whole methodology has been applied, while for the other two, only the first two stages and part of the experiment-based verification stage have been applied, that is, the experimental work has been planned, a list of actions has been generated, but no actual measurement has been taken.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
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An Integrated Systematic Framework to Assist the Development of Pharmaceutical Processes

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Papadakis, E. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
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An optimization based framework for design and retrofit of municipal wastewater treatment plants: Case study on side-stream nitrogen removal technologies
Existing WWTPs need retrofitting due to several different reasons such as: change in the wastewater flow and composition, change in the effluent limits, as well as changes in the wastewater treatment trends. Specifically, increased nitrogen limitations in the regulations for the WWTP effluents gave rise to development of innovative nitrogen removal technologies mostly used for water streams resulting from sludge treatment. In this study we propose a superstructure optimization concept based on mathematical programming to manage the multi-criteria WWTP design/retrofit problem and generate novel and optimal network designs for domestic WWTPs. Alternative treatment technologies are represented in a superstructure; each of which is described by a generic model in terms of input-output mass balances. The superstructure is coupled with a database containing data for both performance and economics of the alternative technologies. The superstructure optimization problem is formulated as a Mixed Integer (Non)Linear Programming problem and solved in GAMS for different scenarios represented by different objective functions and constraint definitions. Finally, a case study is formulated to perform a retrofit study addressing the nitrogen removal problem in order to highlight the use of the framework.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Bozkurt, H. (Intern), Quaglia, A. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

Application of environmental and economic metrics to guide the development of biocatalytic processes
The increasing industrial interest in biocatalytic processes is predominantly driven by the need for selective chemistry, with high reaction yield (Y-reaction) and few side reactions, as well as the need for optically pure chiral molecules (in particular in the pharmaceutical industry). Interestingly, it is often argued that the mild conditions frequently used in biocatalytic reactions (ambient temperature and pressure, neutral pH and aqueous-based media) automatically lead to environmentally-friendly and cost-effective production processes. However, such a conclusion is not justified without the...
use of adequate tools to evaluate the performance of a process, in particular during process development. Nevertheless, at the early development stage, evaluation of biocatalytic processes is not a trivial task, not only due to the lack of data, but also because at this stage many of the biocatalytic processes are not yet fully optimized. Hence, in this paper we propose the use of a range of tools which can be used to guide process development, research tasks and support decision-making. Three sets of metrics are identified, each for use at different stages of process development (route selection, early development and late development), each with different objectives.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Lima Ramos, J. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
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Application of the Generic Modeling Template Approach to Unsaturated Fatty Acid Oxidation and Crystallization Systems.
In this work, a couple of applications of the template-based approach for model development are presented. The computer-aided template concept has been developed based on a model decomposition technique and has been implemented as a software tool, which provides a user-friendly interface for following the modelling workflow steps, guidance through the steps , as well as providing additional information and comments. The application of the tool is highlighted with two case studies: oxidation of unsaturated acid with hydrogen peroxide and modeling of a crystal lization operation for the paracetamol-ethanol system.

General information
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Application of the Generic Modeling Template Approach to Unsaturated Fatty Acid Oxidation and Crystallization Systems.

The computer-aided template concept has been developed based on a model decomposition technique and has been implemented as a software tool, which provides a user-friendly interface for following the modelling workflow steps, guidance through the steps, as well as providing additional information and comments. The purpose of the template approach is to enable the modeller to obtain a general model for a given system, which will be used later to generate problem-specific models. This is based on the idea of the model reuse, which emphasize using a model not only for one specific application but also for future application involving different needs and levels of details to match different purposes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Fedorova, M. (Intern), Papadakis, E. (Intern), Meisler, K. T. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Modeling framework, Computer-aided template, Oxidation of unsaturated fatty acid, Crystallization
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Application of Uncertainty and Sensitivity Analysis to a Kinetic Model for Enzymatic Biodiesel Production

This paper demonstrates the added benefits of using uncertainty and sensitivity analysis in the kinetics of enzymatic biodiesel production. For this study, a kinetic model by Fedosov and co-workers is used. For the uncertainty analysis the Monte Carlo procedure was used to statistically quantify the variability in the model outputs due to uncertainties in the parameter estimates; showing the model is most reliable in the start (first 5 hours) of the reaction. To understand which input parameters are responsible for the output uncertainty, two global sensitivity methods (Standardized Regression Coefficients, and Morris screening) were used. The results from both sensitivity analyses identified that only 10 of the 32 parameters are influential to the model outputs. The model was then simplified by removing the non-influential parameters. A parity plot of the simplified model vs. the full model gave a R2 value of over 0.95 for all the model outputs.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Price, J. A. (Intern), Nordblad, M. (Intern), Woodley, J. (Intern), Huusom, J. K. (Intern)
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A process synthesis-intensification framework for the development of sustainable membrane-based operations

In this paper a multi-level, multi-scale framework for process synthesis-intensification that aims to make the process more sustainable than a base-case, which may represent a new process or an existing process, is presented. At the first level (operation-scale) a conceptual base case design is synthesized through the sequencing of unit operations and subsequently analyzed for identifying process hot-spots using economic, life cycle and sustainability metrics. These hot-spots are limitations/bottlenecks associated with tasks that may be targeted for overall process improvement. At the second level (task-scale) a task-based synthesis method is applied where one or more tasks representing unit operations are identified and analyzed in terms of means-ends for generating intensified flowsheet alternatives. At the third level (phenomena-scale) a phenomena-based synthesis method is applied, where the involved phenomena in various tasks are identified, manipulated and recombined to generate new and/or existing unit operations configured into flowsheet alternatives that target the tasks associated with hot-spots. Every lower-scale or higher-level, generates more alternatives than the corresponding larger-scale. Those alternatives that are able to address the identified hot-spots therefore give innovative and more sustainable process designs that otherwise could not be found from the larger-scales. In this paper, membrane-based operations identified through this framework are highlighted in terms of extension of the combined intensification-synthesis method and its application to generate membrane-based operations. Also, application of the framework is illustrated through a case study involving the production of methyl acetate where membrane-based intensified operations play a major role in determining more sustainable process design alternatives.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Process Engineering and Technology
Authors: Babi, D. K. (Intern), Lutze, P. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.972 SNIP 1.391 CiteScore 2.5
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.979 SNIP 1.518 CiteScore 2.26
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Scopus rating (2010): SJR 0.957 SNIP 1.47
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.873 SNIP 1.457
BFI (2008): BFI-level 1
A Realistic Process Example for MIMO MPC based on Autoregressive Models

Advanced controllers such as model predictive control are in use for a wide range of applications in the process industry. The potential utilization of such advanced predictive controllers is far from exhausted. One barrier for more widespread implementation is the lack of simple methodologies for advanced control design development that may be used by non-experts in control theory. This paper presents and illustrates the use of a simple methodology to design an offset-free MPC based on ARX models. Hence a mechanistic process model is not required. The forced circulation evaporator by Newell and Lee is used to illustrate the offset-free MPC based on ARX models for a nonlinear multivariate process.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
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A Simultaneous Optimization Approach for Synthesis and Design of Process and Water Networks

General information
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A Simultaneous Optimization Approach for Synthesis and Design of Process and Water Networks

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Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences
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A Study of Microalgal Symbiotic Communities with the Aim to Increase Biomass and Biodiesel Production

Microalgae are nearly everywhere and they are responsible for a large part of the world’s primary production. Their ability to grow fast and reach high cell densities makes them candidates for use in the production of biofuel. A key feature of many algae is the production of lipids as storage molecules. A variety of algae can produce large amounts of lipids and these easily be converted to biodiesel for use as transport fuel. Production of algal based biodiesel is however still limited mainly due to production costs. Research is needed in order to lower the price of the final product. In this study interactions between algae and bacteria have been investigated. Many previous investigations have revealed that algae when co-cultured with bacteria reach higher cell numbers and exhibit faster growth rates. Part of the study focuses on interactions between the green algae Dunaliella salina and three strains of bacteria, Pelagibaca, Halomonas and Marinobacter, isolated from the algal culture. Growing axenic D. salina in co-culture with the bacteria results in markedly higher cell densities. Another part of the study focuses on interactions between three strains of Scenedesmus like algae, isolated water samples obtained locally, and bacteria from one of the water samples. Interestingly the three closely related algae react very differently to being co-cultured with the bacteria. One algal strain is unaffected, one is promoted in growth, and one is negatively affected. In the final part of the study the effect of hypo and hyper-saline shock on D. salina was investigated. Theoretically D. salina would produce lipids when stressed however no appearance of lipids was detected in the cells subjected to a hypo-saline shock and in the case of a hyper-saline shock lipids could be detected early on but disappeared within 48 h.

General information
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Authors: Baggesen, C. (Intern), Gjermansen, C. (Intern), Brandt, A. B. (Intern)
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A systematic methodology for design of tailor-made blended products

A systematic methodology for design of tailor-made blended products has been developed. In tailor-made blended products, one identifies the product needs and matches them by blending different chemicals. The systematic methodology has four main tasks. First, the design problem is defined: the product needs are identified, translated into target properties and the bounds for each target property are defined. Secondly, target property models are retrieved from a property model library. Thirdly, a mixture/blend design algorithm is applied to obtain the mixtures/blends that match the design targets. The result is a set of blends that match the constraints, the composition of the chemicals present in the blend, and the values of the target properties. Finally, the mixture target property values are verified by means of rigorous models for the properties and the mixtures. In this paper, the methodology is highlighted through two case studies involving gasoline blends and lubricant base oils.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. B. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
A Tuning Approach for Offset-free MPC with Conditional Reference Adaptation.

Model predictive control has become a widely accepted strategy in industrial applications in the recent years. Often mentioned reasons for the success are the optimization based on a system model, consideration of constraints and an intuitive tuning process. However, as soon as unknown disturbances or model plant mismatch have to be taken into account the tuning effort to achieve offset-free tracking increases. In this work a novel approach for offset-free MPC is presented, which divides the tuning in two steps, the setup of a nominal MPC loop and an external reference adaptation. The inner nominal loop addresses the performance targets in the nominal case, decouples the system and essentially leads to a first order response. The second outer loop enables offset-free tracking in case of unknown disturbances and consists of feedback controllers adapting the reference. Due to the mentioned properties these controllers can be tuned separate and by known guidelines. To address conditions with active input constraints, additionally a conditional reference adaptation scheme is introduced. The tuning strategy is evaluated on a simulated linear Wood-Berry binary distillation column example.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Johannes Kepler University of Linz
Authors: Waschl, H. (Ekstern), Jørgensen, J. B. (Intern), Huusom, J. K. (Intern), del Re, L. (Ekstern)
Pages: 3062-3067
Publication date: 2014

Balancing effluent quality, economic cost and greenhouse gas emissions during the evaluation of (plant-wide) control/operational strategies in WWTPs

The objective of this paper was to show the potential additional insight that result from adding greenhouse gas (GHG) emissions to plant performance evaluation criteria, such as effluent quality (EQI) and operational cost (OCI) indices, when evaluating (plant-wide) control/operational strategies in wastewater treatment plants (WWTPs). The proposed GHG evaluation is based on a set of comprehensive dynamic models that estimate the most significant potential on-site and off-site sources of CO2, CH4 and N2O. The study calculates and discusses the changes in EQI, OCI and the emission of GHGs as a consequence of varying the following four process variables: (i) the set point of aeration control in the activated sludge section; (ii) the removal efficiency of total suspended solids (TSS) in the primary clarifier; (iii) the temperature in the anaerobic digester; and (iv) the control of the flow of anaerobic digester supernatants coming from sludge treatment. Based upon the assumptions built into the model structures, simulation results highlight the potential undesirable effects of increased GHG production when carrying out local energy optimization of the aeration system in the activated sludge section and energy recovery from the AD. Although off-site CO2 emissions may decrease, the effect is counterbalanced by increased N2O emissions, especially since N2O has a 300-fold stronger greenhouse effect than CO2. The reported results emphasize the importance and usefulness of using multiple evaluation criteria to compare and evaluate (plant-wide) control strategies in a WWTP for more informed operational decision making. © 2013 Elsevier B.V.

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Batch production of FAEE-biodiesel using a liquid lipase formulation

The application of lipase catalysis to the production of biodiesel has received much interest during the past several years. Although most of the previous work has involved the use of immobilized enzyme, more recent work has indicated that liquid formulations of lipase can provide a highly competitive option for the conversion of oils and fats to biodiesel. This study investigates the impact of several process parameters on the production of fatty acid ethyl esters from rapeseed oil in a pure batch process on the liquid lipase formulation Callera™ Trans L. Oil conversion in excess of 98% was achieved by combining a 50% stoichiometric excess of ethanol (1.5 equivalents) with 20% (w/w) water relative to the oil. The rate of reaction was directly proportional to the amount of lipase added in this system (500-2000 LU per gram oil). Addition of glycerol to the initial reaction mixture reduced the initial reaction rate, but also improved the final yield of biodiesel by suppressing hydrolysis. © 2014 Published by Elsevier B.V.
Biodiesel production, Fatty acid ethyl esters, Transesterification, Lipase catalysis, Process evaluation, Batch data processing, Catalysis, Esterification, Esters, Fatty acids, Liquids, Fatty acid ethyl ester, Immobilized enzyme, Liquid formulations, Process Evaluation, Process parameters, Reaction mixture, Biodiesel

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Benchmarking of Control Strategies for Wastewater Treatment Plants

Wastewater treatment plants are large non-linear systems subject to large perturbations in wastewater flow rate, load and composition. Nevertheless these plants have to be operated continuously, meeting stricter and stricter regulations. Many control strategies have been proposed in the literature for improved and more efficient operation of wastewater treatment plants. Unfortunately, their evaluation and comparison – either practical or based on simulation – is difficult. This is partly due to the variability of the influent, to the complexity of the biological and biochemical phenomena and to the large range of time constants (from a few minutes to several days). The lack of standard evaluation criteria is also a tremendous disadvantage. To really enhance the acceptance of innovative control strategies, such an evaluation needs to be based on a rigorous methodology including a simulation model, plant layout, controllers, sensors, performance criteria and test procedures, i.e. a complete benchmarking protocol.

General information
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Organisations: Department of Environmental Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universite Laval, McMaster University, Lund University
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Number: 23
Main Research Area: Technical/natural sciences
Biocatalytic process development using microfluidic miniaturized systems

The increasing interest in biocatalytic processes means there is a clear need for a new systematic development paradigm which encompasses both protein engineering and process engineering. This paper argues that through the use of a new microfluidic platform, data can be collected more rapidly and integrated with process modeling, can provide the basis for validating a reduced number of potential processes. The miniaturized platform should use a smaller reagent inventory and make better use of precious biocatalysts. The EC funded BIOINTENSE project will use ω-transaminase based synthesis of chiral amines as a test-bed for assessing the viability of such a high throughput biocatalytic process development, and in this paper, such a vision for the future is presented.

Bioprocess engineering for the application of P450s

The highly specific hydroxylation performed by P450 monoxygenases is a very powerful tool for synthetic chemists, not only at laboratory scale, but potentially also at industrial scale. However, despite this potential, only in a few cases has this class of enzymes been implemented at an industrial scale. In the case of P450s, the requirements for cofactor and electron transporting redox partner, coupled with conversion of hydrophobic substrates to hydrophobic products already set some constraints. In order to enable focused and directed improvement of the biocatalyst (and process), such limitations need to be quantified via carefully designed experiments. In this presentation, we will report the results of a hypothesis driven experimental approach to characterization, with the aim of quantifying the limitations associated with cofactor regeneration, inhibition, toxicity and trans-membrane transport. Selected test reactions and biocatalysts made available within the EC FP7 research program P4FIFTY have been used for the study, including CYP153A[1], CYP102A1[2] expressed in Escherichia coli and CYP106A2[3] expressed in Bacillus megaterium. Common limitations have been found to be the stability of the biocatalyst, as well as substrate inhibition and toxicity. These limitations will influence what we have reported as typical targets necessary to implement a commercially feasible process (reaction yield, biocatalyst yield, final product concentration and space-time yield). The analysis reveals that while further improvements are required to reach the targets, the remaining limitations should ultimately be possible to overcome. Such a process analysis tool can in principle be applied to many biocatalytic systems and it is hoped that in the future it will help to enable accelerated biocatalytic process development.
Calibration and validation of a phenomenological influent pollutant disturbance scenario generator using full-scale data

The objective of this paper is to demonstrate the full-scale feasibility of the phenomenological dynamic influent pollutant disturbance scenario generator (DIPDSG) that was originally used to create the influent data of the International Water Association (IWA) Benchmark Simulation Model No. 2 (BSM2). In this study, the influent characteristics of two large Scandinavian treatment facilities are studied for a period of two years. A step-wise procedure based on adjusting the most sensitive parameters at different time scales is followed to calibrate/validate the DIPDSG model blocks for: 1) flow rate; 2) pollutants (carbon, nitrogen); 3) temperature; and, 4) transport. Simulation results show that the model successfully describes daily/weekly and seasonal variations and the effect of rainfall and snow melting on the influent flow rate, pollutant concentrations and temperature profiles. Furthermore, additional phenomena such as size and accumulation/flush of particulates of/in the upstream catchment and sewer system are incorporated in the simulated time series. Finally, this study is complemented with: 1) the generation of additional future scenarios showing the effects of different rainfall patterns (climate change) or influent biodegradability (process uncertainty) on the generated time series; 2) a demonstration of how to reduce the cost/workload of measuring campaigns by filling the gaps due to missing data in the influent profiles; and, 3) a critical discussion of the presented results balancing model structure/calibration procedure complexity and prediction capabilities.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University, Copenhagen Wastewater Innovation
Authors: Flores Alsina, X. (Intern), Saagi, R. (Ekstern), Lindblom, E. U. (Ekstern), Thirsing, C. (Ekstern), Thornberg, D. (Ekstern), Gernaey, K. V. (Intern), Jeppsson, U. (Ekstern)
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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
General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern), Woodley, J. (Intern)
Number of pages: 79
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Publication information
Publisher: Technical University of Denmark, Department of Chemical and Biochemical Engineering
Original language: English
Main Research Area: Technical/natural sciences
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Challenges encountered when expanding activated sludge models: a case study based on N2O production.
It is common practice in wastewater engineering to extend standard activated sludge models (ASMs) with extra process equations derived from batch experiments. However, such experiments have often been performed under conditions different from the ones normally found in wastewater treatment plants (WWTPs). As a consequence, these experiments might not be representative for full-scale performance, and unexpected behaviour may be observed when simulating WWTP models using the derived process equations. In this paper we want to highlight problems encountered using a simplified case study: a modified version of the Activated Sludge Model No. 1 (ASM1) is upgraded with nitrous oxide (N2O) formation by ammonia-oxidizing bacteria. Four different model structures have been implemented in the Benchmark Simulation Model No. 1 (BSM1). The results of the investigations revealed two typical difficulties: problems related to the overall mathematical model structure and problems related to the published set of parameter values. The paper describes the model implementation incompatibilities, the variability in parameter values and the difficulties of reaching similar conditions when simulating a full-scale activated sludge plant. Finally, the simulation results show large differences in oxygen uptake rates, nitritation rates and consequently the quantity of N2O emission (G(N2O)) using the different models.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University
Authors: Snip, L. (Intern), Boiocchi, R. (Intern), Flores Alsina, X. (Intern), Jeppsson, U. (Ekstern), Gernaey, K. (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 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
Challenges in industrial fermentation technology research

Industrial fermentation processes are increasingly popular, and are considered an important technological asset for reducing our dependence on chemicals and products produced from fossil fuels. However, despite their increasing popularity, fermentation processes have not yet reached the same maturity as traditional chemical processes, particularly when it comes to using engineering tools such as mathematical models and optimization techniques. This perspective starts with a brief overview of these engineering tools. However, the main focus is on a description of some of the most important engineering challenges: scaling up and scaling down fermentation processes, the influence of morphology on broth rheology and mass transfer, and establishing novel sensors to measure and control insightful process parameters. The greatest emphasis is on the challenges posed by filamentous fungi, because of their wide applications as cell factories and therefore their relevance in a White Biotechnology context. Computational fluid dynamics (CFD) is introduced as a promising tool that can be used to support the scaling up and scaling down of bioreactors, and for studying mixing and the potential occurrence of gradients in a tank. © 2014 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

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Journal: Biotechnology Journal
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.172 SNIP 0.874 CiteScore 2.91
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.189 SNIP 1.062 CiteScore 2.98
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.136 SNIP 1.093 CiteScore 3.01
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.944 SNIP 0.957 CiteScore 2.4
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.785 SNIP 0.726 CiteScore 1.94
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.787 SNIP 0.798
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.695 SNIP 0.749
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.581 SNIP 0.806
Scopus rating (2007): SJR 0.568 SNIP 0.709
Web of Science (2007): Indexed yes
Original language: English
Computational fluid dynamics, Fermentation process development, Fungal morphology, Industrial biotechnology, Modeling, Scale-down bioreactors, Bioreactors, Biotechnology, Fermentation, Industry, Mathematical models, Models, Morphology, Process control, Engineering challenges, Fermentation process, Industrial fermentation, Measure and controls, Optimization techniques, Scale-down, Industrial chemicals
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ChemBioTec - Linking chemistry, biology and engineering

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Osnabrück, Technical University of Dortmund
Authors: Heiden, S. (Ekstern), Heiden, F. (Ekstern), Woodley, J. (Intern), Schmid, A. (Ekstern)
Number of pages: 1
Publication date: 2014
Main Research Area: Technical/natural sciences

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Journal: Journal of Molecular Catalysis B: Enzymatic
Comparison of techniques for reconstruction of a distribution from moments in the context of a pharmaceutical drying process

The use of moment-based methods to solve a Population Balance Model (PBM) induces the need to reconstruct a distribution from the moments for system analysis. Several reconstruction methods are investigated (i.e. parameter fitting methods and the method of splines), compared with each other as well as with the result of a non-moment-based solution method for the PBM. The finetuning of the parameters for the method of splines was very important for the final result as well as for the computational time. An additional parameter, i.e. a different value for the first and the last interval for toler, was introduced to improve the result and speed up the calculation. None of the parameter fitting methods was able to correctly predict several peaks in the final distribution. In contrast, the method of splines was able to reconstruct the distribution even without prior knowledge. However, prior knowledge about the distribution does facilitate the finetuning. © 2014 Elsevier Ltd.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Ghent University
Authors: Mortier, S. T. F. (Ekstern), De Beer, T. (Ekstern), Gernaey, K. V. (Intern), Nopens, I. (Ekstern)
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BFI (2017): BFI-level 2
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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
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
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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
Computer-Aided framework for Sustainable Process Design - targeting conceptual and detailed engineering phases

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Utrecht University
Authors: Loureiro da Costa Lira Gargalo, C. (Intern), Duque, J. P. (Ekstern), Sin, G. (Intern)
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences

Bibliographical note
ORAL PRESENTATION
Source: PublicationPreSubmission
Source-ID: 103645239
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Computer-Aided Template for Model Reuse, Development and Maintenance
A template-based approach for model development is presented in this work. Based on a model decomposition technique, 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, as well as the guidance through the steps providing additional information and comments. The application of the tool is highlighted with a multiscale modeling case study involving a catalytic membrane fixed bed reactor. The modeling templates for reactor as well as particle scales have been developed. For the particle scale, two alternative mechanisms to describe the diffusion inside catalyst pellets are available: a Fickian diffusion model and a dusty gas model. Moreover, the effects of isothermal and non-isothermal catalyst are also considered during the model development process. Thereby, any number of problem-specific models can be generated through the template and maintained for the future reuse.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Conditional Reference Adaptation for Offset-free MPC

Model predictive control has become a widely accepted strategy in industrial applications in the recent years. Often mentioned reasons for the success are the optimization based on a system model, consideration of constraints and an intuitive tuning process. However, as soon as unknown disturbances or model plant mismatch have to be taken into account the tuning effort to achieve offset-free tracking increases. In this work a novel approach for offset-free MPC is presented, which divides the tuning in two steps, the setup of a nominal MPC loop and an external reference adaptation. The inner nominal loop addresses the performance targets in the nominal case, decouples the system and essentially leads to a first order response. The second outer loop enables offset-free tracking in case of unknown disturbances and consists of feedback controllers adapting the reference. Due to the mentioned properties these controllers can be tuned separate and by known guidelines. To address conditions with active input constraints, additionally a conditional reference adaptation scheme is introduced. The tuning strategy is evaluated on a simulated linear Wood-Berry binary distillation column example.

Consistent thermodynamic properties of lipids systems

Physical and thermodynamic properties of pure components and their mixtures are the basic requirement for process design, simulation, and optimization. In the case of lipids, our previous works[1-3] have indicated a lack of experimental data for pure components and also for their mixtures. To contribute in this area, experimental data were obtained using the Differential Scanning Calorimetry (DSC) technique for isobaric vapor-liquid equilibrium (VLE) of two binary mixtures at two different pressures (1.2 and 2.5 KPa): system 1 [monoacylglycerol (monocaprylin) + fatty acid (palmitic acid)] and system 2 [monoacylglycerol (monocaprylin) + fatty ester (methyl stearate)]. System 1 is relevant in the purification steps of the deodorizer distillates while system 2 is relevant in the purification steps of biodiesel and bioglycerin. A non-ideal behavior is revealed for both systems at the two different pressures, with azeotrope behavior observed. Available thermodynamic consistency tests for TPx data were applied before performing parameter regressions for Wilson, NRTL, UNIQUAC and original UNIFAC models. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC model. For solid-liquid equilibrium (SLE) data, new consistency tests have been developed [2]. Some of the developed tests were based in the quality tests proposed for VLE data by Kang et al. [4] and a methodology that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions are discussed. In this work, case studies considering the methodology proposed for SLE thermodynamic consistency tests and data from open literature and databases such as NIST-TDE®, DIPPR® and DECHEMA® are presented. The SLE consistency test and data evaluation is performed in a software containing option for
Consistent vapour-liquid equilibrium data containing lipids

Consistent physical and thermodynamic properties of pure components and their mixtures are important for process design, simulation, and optimization as well as design of chemical based products. In the case of lipids, it was observed a lack of experimental data for pure compounds and also for their mixtures in open literature, what makes necessary the development of reliable predictive models based on limited data. To contribute to the missing data, measurements of isobaric vapour-liquid equilibrium (VLE) data of three binary mixtures at two different pressures were performed at State University of Campinas (UNICAMP – Brazil), using Differential Scanning Calorimetry (DSC) technique, i.e., monoacylglycerol + fatty acid (system 1), monoacylglycerol + fatty ester (system 2) and monoacylglycerol + glycerol (system 3). System 1 is relevant in the purification steps of the deodorizer distillates while systems 2 and 3 are relevant in the purification steps of biodiesel and bioglycerin. It should be highlighted that there is no such data in the open literature, not only for the specific compounds we selected but also for the combination of the classes of compounds considered in this work. Available thermodynamic consistency tests for TPx data were applied before performing parameter regressions for well-known thermodynamic models such as Wilson, NRTL, UNIQUAC and UNIFAC. In the pure compound consistency test (Qtest,5 of TDE program developed at NIST), the consistencies of the end-points (x=0 and 1) of the VLE data are considered by comparing these values with their pure compound vapor pressures. Van Ness test where also considered in this work (Qtest,1 of program TDE developed at NIST), that check how the measured data represent the thermodynamic models. Boiling temperatures and vapor phase compositions were calculated using Wilson, NRTL, UNIQUAC, and original UNIFAC models and bubble-point calculations. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC model and by proposing new interaction parameters for UNIFAC model and lipids systems. Also PC-SAFT model were analysed for lipids and a modification is proposed.
Control Benchmark for Solvent Recovery by Distillation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
Authors: Lützen, P. (Ekstern), Mauricio Iglesias, M. (Intern), Huusom, J. K. (Intern), Abildskov, J. (Intern)
Publication date: 2014
Event: Abstract from 10th International Conference on Distillation and Absorption 2014, Friedrichshafen, Germany.
Main Research Area: Technical/natural sciences

Cost Estimation for Early-Stage Synthesis and Design of Biorefinery Networks

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Cheali, P. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences

Crystallization Kinetics within a Generic Modeling Framework

A new and extended version of a generic modeling framework for analysis and design of crystallization operations is presented. The new features of this framework are described, with focus on development, implementation, identification, and analysis of crystallization kinetic models. Issues related to the modeling of various kinetic phenomena like nucleation, growth, agglomeration, and breakage are discussed in terms of model forms, model parameters, their availability and/or estimation, and their selection and application for specific crystallization operational scenarios under study. The advantages of employing a well-structured model library for storage, use/reuse, and analysis of the kinetic models are highlighted. Examples illustrating the application of the modeling framework for kinetic model discrimination related to simulation of specific crystallization scenarios and for kinetic model parameter estimation are presented.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS
Authors: Meisler, K. T. (Intern), von Solms, N. (Intern), Gernaey, K. V. (Intern), Gani, R. (Intern)
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BFI (2016): BFI-level 1
Data Driven Modeling for Monitoring and Control of Industrial Fed-Batch Cultivations

A systematic methodology for development of a set of discrete-time sequence models for batch control based on historical and online operating data is presented and investigated experimentally. The modeling is based on the two independent characteristic time dimensions of batch processing, being time within the batch and the batch number. The model set is parsimoniously parametrized as a set of local, interdependent models which are estimated from data for as few as half a dozen batches. On the basis of state space models transformed from the acquired input-output model set, the asymptotic convergence of iterative learning control is combined with the closed-loop performance of model predictive control to form an optimal controller aiming to ensure reliable and reproducible operation of the batch process. This learning model predictive controller may also be used for optimizing control through optimization of the bioreactor operations model. The modeling and preliminary control performance is demonstrated on an industrial fed-batch protein cultivation production process. The presented methods lend themselves directly for application as Process Analytical Technologies.
Development and analysis of the Original UNIFAC-CI model for prediction of vapor–liquid and solid–liquid equilibria

In this work, we present a further development and analysis of the Original UNIFAC-CI models for the prediction of vapor–liquid equilibrium (VLE) and solid–liquid equilibrium (SLE) for a wide range of mixtures. Three sets of atom interaction parameters (AIPs) have been regressed. For the first two sets, only VLE experimental data were used in parameter estimation. In the first set, no weighting factors were used for each of the VLE data in the objective function when regressing the AIPs. However, for the second set, the AIPs have been regressed using the so-called QVLE quality factors obtained for each of the VLE data from a quality assessment algorithm (consistency tests) as weighting factors in the objective functions. For the third set of parameters, SLE and VLE data were used in the regression of AIPs. The result of the correlations in terms of deviations errors and predictions using these three sets of regressed parameters are presented, compared and discussed. The significance of adding the QVLE values and SLE systems in the regression of the AIPs are also highlighted. UNIFAC is a model that can be in principle used for both VLE and SLE (as well as other types of phase behavior) calculations. The range of applicability of the predictive UNIFAC-CI is investigated and it is shown to what extent the Original UNIFAC-CI model can successfully predict SLE especially when the needed parameters are missing.
Development of novel control strategies for single-stage autotrophic nitrogen removal: A process oriented approach

The autotrophic nitrogen removing granular sludge process is a novel and intensified process. However, its stable operation and control remain a challenging issue. In this contribution, a process oriented approach was used to develop, evaluate and benchmark novel control strategies to ensure stable operation and rejection of disturbances. Three novel control strategies were developed, evaluated, and benchmarked against each other: a feedforward control (control structure 1 – CS#1), a rule-based feedback control (CS#2), and a feedforward–feedback controller, in which the feedback loop updates the set point of the feedforward loop (CS#3). The CS#1 gave the best performance against disturbances in the ammonium concentration, whereas the CS#2 provided the best performance against disturbances in the organic carbon concentration and dynamic influent conditions. The CS#3 rejected both disturbances satisfactorily. Thus, the appropriate design will depend on the specific disturbances in the influent generated in the upstream units of the wastewater treatment plant.
Dynamic data evaluation for solid-liquid equilibria

The accuracy and reliability of the measured data sets to be used in regression of model parameters is an important issue related to modeling of phase equilibria. It is clear that good parameters for any model cannot be obtained from low quality data. A thermodynamic consistency test for solid-liquid systems using a relation between the solid and liquid activity coefficients for systems containing metals [1], where the data from the two phases are given were proposed. However, as consistency tests based on the Gibbs–Duhem equation are not feasible, new consistency tests have been developed [2]. Some of the developed tests were based in the quality tests proposed for VLE data by Kang et al. [3] and a methodology that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions are discussed. In this work, case studies considering the methodology proposed for SLE thermodynamic consistency tests and data from open literature and databases such as NIST-TDE®, DIPPR® and DECHEMA® are presented. The SLE consistency test and data evaluation is performed in a software containing option for data analysis, model analysis and parameter regression. The paper will highlight the data collection, the data analysis for SLE data and the thermodynamic model performance (such as NRTL, UNIQUAC and original UNIFAC).

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 digester 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.
Dynamic Simulation, Sensitivity and Uncertainty Analysis of a Demonstration Scale Lignocellulosic Enzymatic Hydrolysis Process

This study presents the uncertainty and sensitivity analysis of a lignocellulosic enzymatic hydrolysis model considering both model and feed parameters as sources of uncertainty. The dynamic model is parametrized for accommodating various types of biomass, and different enzymatic complexes, accounting a large number of parameters. The sensitivity analysis of model predictions with respect to model parameters is quantified by the delta mean square measure. By ranking the delta mean square, a reduced subset of parameters is found helping to identify the bottleneck of the model. The uncertainty analysis is carried for both model parameters and feed composition in order to assess the accuracy of the predictions. First, the model and feed parameters are sampled by Latin Hypercube Sampling (LHS) and then Monte Carlo simulations are run with the sampled values. Feed parameters are considered to be affected by non-zero mean noise because they are determined by a Near Infrared (NIR) instrument. LHS is performed on 2 parameters: the probability of the mean value and the probability of the standard deviation for each measurement. The Monte Carlo outputs are then analyzed by linear regression and the standardized regression coefficients (SRC) are computed for identifying the responsible parameters for model outputs precision. It is found that sugar yields are mostly sensitive to the composition of the enzymatic complex, and xylooligomers and glucose inhibition. pH is affected mostly by the amount of acetyl groups in the hemicellulose, while viscosity is sensitive to a few coefficients from its empirical equation.

General information
State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Prunescu, R. M. (Intern), Sin, G. (Intern)
Number of pages: 11
Publication date: 2014

Early-Stage Bioprocess Analysis (ESBA)
Biocatalysis encompasses the use of enzymes or whole cell systems for effecting the conversion of readily available, inexpensive starting materials to high value products. Enzymes are fully recyclable catalytic proteins that frequently display exquisite chemo-, enantio- and regioselectivity and operate under mild conditions of pH and temperature. These characteristics make them cost-effective and sustainable catalysts for a wide range of chemical transformations. Modern tools of protein discovery and engineering as well as advances in molecular biology and protein structure aid the development of biocatalysts and their tailor-designed integration into industrial processes. Consequently, they find wide application in the production of pharmaceutical intermediates, novel materials and diagnostics, as well as fine, performance and commodity chemicals. The Biocatalysis Gordon Research Conference highlights the best science, technologies and case studies to provide in-depth understanding of the development and practical use of biocatalysts.
around the world.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Seita, C. S. (Intern), Rehdorf, J. (Ekstern), Woodley, J. (Intern)
Number of pages: 1
Publication date: 2014
Event: Abstract from Gordon Research Seminar (GRS) on Biocatalysis, Smithfield, RI, United States.
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 128756776
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

**Early Stage Design of a Bio refinery from Castor Oil.**
This paper presents a systematic method for synthesis and analysis of bio mass based biorefinery pathways (process networks) in terms of current and future market conditions. The systematic method has been implemented into a computer aided tool that is able to quickly evaluate alternatives and network scenarios. The tool integrates data collection, modelling and superstructure optimization to determine the optimal network for a biorefinery. The application of the synthesis - analysis method and its corresponding computer aided tool is highlighted for a case study where castor oil is the specified biomass available for the biorefinery.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CAPEC-PROCESS, Universidade Federal do Rio de Janeiro
Authors: de Faria, D. (Ekstern), Quaglia, A. (Intern), Pessoa, F. (Ekstern), Gani, R. (Intern)
Pages: 489-494
Publication date: 2014

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Main Research Area: Technical/natural sciences
Castor oil, Superstructure optimization, Integrated business and engineering framework, Separation process synthesis
Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

**Early-stage design of municipal wastewater treatment plants – presentation and discussion of an optimisation based concept**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Bozkurt, H. (Intern), Quaglia, A. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Number of pages: 1
Publication date: 2014
Event: Poster session presented at 4th IWA/WEF Wastewater Treatment Modelling Seminar 2014, Spa, Belgium.
Main Research Area: Technical/natural sciences
Design, Modelling, Superstructure optimization, Uncertainty, Wastewater treatment
Electronic versions: WWTmod_PosterHB.pdf
Source: PublicationPreSubmission
Source-ID: 102161538
Publication: Research - peer-review › Poster – Annual report year: 2014
Early-stage design of municipal wastewater treatment plants – presentation and discussion of an optimisation based concept

The number of alternative WWT technologies has grown steadily to meet increasingly stringent performance demands which increased the importance and complexity of early-stage decision making in WWTP design and retrofitting problems. Currently the conceptual design task is handled based on expert decisions and previous experiences. In this contribution, we propose a new approach based on mathematical programming to manage the complexity of the problem and generate novel and optimal WWTP network designs for domestic WWT. Within this context, a superstructure concept is used to represent the alternative WWT technologies described as a series of reaction and separation tasks at different treatment levels. Each process alternative is described by a generic model and the required data for both performance and economics of each alternative are collected and sorted in a multi-dimensional database. This database is embedded within the mixed integer nonlinear programming problem formulated and solved in GAMS for different objective functions (e.g., total annualized costs, etc.) and constraint definitions (e.g., effluent discharge limits). The developed framework is highlighted using the benchmark plant as a case study to generate and screen optimal concepts for retrofitting options under different scenarios.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Bozkurt, H. (Intern), Quaglia, A. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Pages: 254-257
Publication date: 2014

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Main Research Area: Technical/natural sciences
Conference: 4th IWA/WEF Wastewater Treatment Modelling Seminar 2014, Spa, Belgium, 30/03/2014 - 30/03/2014
Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

Editorial note for the Best Paper of 2012 Award

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Columbia University
Authors: Venkatasubramanian, V. (Ekstern), Gani, R. (Intern)
Pages: iii-iv
Publication date: 2014
Main Research Area: Technical/natural sciences

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BFI (2016): BFI-level 2
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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
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
This paper presents the development of a computer-aided decision support tool for identifying optimal biorefinery concepts for production of biofuels at an early design stage. To this end, a framework that uses a superstructure-based process synthesis approach integrated with uncertainty analysis is used. We demonstrate the application of the tool for generating optimal biorefinery concepts for a lignocellulosic biorefinery. In particular, we highlight the management of various sources of data, the superstructure (integrated thermochemical and biochemical conversion routes) needed to represent the design space, generic but simple models describing the processing tasks, and the formulation and solution of an MINLP problem under deterministic and stochastic conditions to identify the optimal processing route for multiple raw materials and products. Furthermore, we evaluate the impact of market price uncertainties on the optimal solutions and calculate the associated risk to enable informed and risk-aware decisions.

**General information**
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
- **Authors:** Cheali, P. (Intern), Quaglia, A. (Intern), Gernaey, K. V. (Intern), Sin, G. (Intern)
- **Pages:** 6021-6032
- **Publication date:** 2014
- **Main Research Area:** Technical/natural sciences
Effects of ion strength and ion pairing on (plant-wide) modelling of anaerobic digestion processes

The objective of this study is to show the influence of ionic strength (as activity corrections) and ion pairing on (plant-wide) modelling of anaerobic digestion processes in wastewater treatment plants (WWTPs). Using the Benchmark Simulation Model No. 2 (BSM2) as a case study, this paper presents the effects that an improved physico-chemical description will have on the predicted effluent quality (EQI) and operational cost (OCI) indices. The acid-base equilibria implemented in the Anaerobic Digestion Model No. 1 (ADM1) are modified to account for non-ideal aqueous-phase chemistry. The model corrects for ionic strength via the Davies approach to consider chemical activities instead of molar concentrations. Also, a speciation sub-routine based on a multi-dimensional Newton-Raphson iteration method accounts for the formation of some of the ion pairs playing an important role in wastewater treatment processes. Results at high ionic strength demonstrate that corrections to account for non-ideal conditions lead to significant differences in predicted process performance. In addition, the paper describes: 1) how the anaerobic digester performance is affected; 2) the effect on pH and the anaerobic digestion products (CO₂, CH₄, and H₂); and, 3) how these variations are propagated from the sludge treatment to the water line.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Queensland, Lund University, Ghent University
Authors: Flores-Alsina, X. (Intern), Mbamba, C. K. (Ekstern), Solon, K. (Ekstern), Volcke, E. (Ekstern), Tait, S. (Ekstern), Batstone, D. (Ekstern), Gernaey, K. V. (Intern), Jeppsson, U. (Ekstern)
Number of pages: 9
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Source: PublicationPreSubmission
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Engineering of Biocatalysts and Biocatalytic Processes
Discovering and developing new biocatalytic reactions and biocatalysts has been the major focus of the activities in the EC FP7 BIOTRAINS network. However, industrial implementation of these new reactions requires engineering of both the biocatalysts and the associated processes, to achieve the necessary targets for economic and sustainable feasibility of full-scale processes. The possible engineering solutions can most rapidly be identified using a series of tools and in this article we will describe some of these as well as giving a perspective on the future of this important element of process research and development.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Lima Ramos, J. (Intern), Lima Afonso Neto, W. (Intern), Woodley, J. (Intern)
Pages: 301-320
Publication date: 2014
Main Research Area: Technical/natural sciences

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Journal: Topics in Catalysis
Volume: 57
Issue number: 5
ISSN (Print): 1022-5528
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BFI (2018): BFI-level 1
Enzymatically Assisted CO$_2$ Removal from Flue-Gas

The enzyme carbonic anhydrase is an enzyme known to enhance CO2 absorption rates. However, for economic viability in enzyme based absorption technology long term stability under process relevant conditions is needed. Thus, here
enzyme stability for extended times are investigated with respect to pH, temperature and solvent. Temperatures and pH stability were tested for up to 100 hours incubation and the enzyme was temperature stable up to 60 °C and in the pH range from 7 to 11, with some residual activity between pH 5 and 12. Furthermore, enzyme stability was tested for 7 different capture solvents for 150 days, at 1 M or 3 M solvent concentrations, 40 °C and pH between 8-9 and 10. Residual activity was found with all samples ranging from 12 to 91 % of the initial activity. This study show that this enzyme can indeed be used for extended periods in process relevant conditions, and thus shows promise for industrial implementation as a catalyst in carbon capture.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Gundersen, M. T. (Intern), von Solms, N. (Intern), Woodley, J. (Intern)
Pages: 624 – 632
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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
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- 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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**Enzyme characterisation in microreactors by multivariate data analysis**
Fed-Batch Feeding Strategies for Enzymatic Biodiesel Production

In this work a kinetic model for the enzymatic transesterification of rapeseed oil using a solubilised lipase (Callera Trans L-Thermomyces lanuginosus) was developed from first principles. The model is based on a Ping-Pong Bi-Bi mechanism, with methanol inhibition, along with consideration of the differences in the interfacial and bulk concentrations of the enzyme. The model is then used to evaluate various feeding strategies to improve the enzymatic biodiesel production. The feeding strategies investigated, gave insight into how the methanol should be fed to potentially mitigate enzyme deactivation while improving the biodiesel yield. The best experimental results gave a yield of 703.76 g FAME L-1 and a reactor productivity of 28.12 g FAME L-1 h-1. In comparison, to reach the same yield, the optimised two step feeding strategy took 6.25 hours less, which equates to an increase the reactor productivity of 36.9%.
Filamentous Fungi Fermentation

Filamentous fungi (including microorganisms such as Aspergillus niger and Rhizopus oryzae) represent an enormously important platform for industrial fermentation. Two particularly valuable features are the high yield coefficients and the ability to secrete products. However, the filamentous morphology, together with non-Newtonian rheological properties (shear thinning), result in poor oxygen transfer unless sufficient energy is provided to the fermentation. While genomic research may improve the organisms, there is no doubt that to enable further application in future it will be necessary to match such research with studies of oxygen transfer and energy supply to high viscosity fluids. Hence, the implementation of innovative solutions (some of which in principle are already possible) will be essential to ensure the further development of such fermentations.

Financial risk analysis in the synthesis and design of processing networks: Balancing risk and return

The construction of a processing network is a corporate investment, that processing companies make with the goal of creating the conditions to increase their value. In a previous work, a computer-aided framework supporting the design of processing network under uncertainty has been presented (Quaglia et al. 2013). In this contribution, we study the implications of corporate finance concepts such as funding strategies and cost of the capital on the selection of an optimal processing network. To this end, the process synthesis framework is extended to include various project funding and financial risk models. Through the solution of a small benchmark problem, the impact of financial factors on the optimal network configuration is presented and discussed.
Generation of (synthetic) influent data for performing wastewater treatment modelling studies

The success of many modelling studies strongly depends on the availability of sufficiently long influent time series - the main disturbance of a typical wastewater treatment plant (WWTP) - representing the inherent natural variability at the plant inlet as accurately as possible. This is an important point since most modelling projects suffer from a lack of realistic data representing the influent wastewater dynamics. The objective of this paper is to show the advantages of creating synthetic data when performing modelling studies for WWTPs. This study reviews the different principles that influent generators can be based on, in order to create realistic influent time series. In addition, the paper summarizes the variables that those models can describe: influent flow rate, temperature and traditional/emerging pollution compounds, weather conditions (dry/wet) as well as their temporal resolution (from minutes to years). The importance of calibration/validation is addressed and the authors critically analyse the pros and cons of manual versus automatic and frequentistic vs Bayesian methods. The presentation will focus on potential engineering applications of influent generators, illustrating the different model concepts with case studies. The authors have significant experience using these types of tools and have worked on interesting case studies that they will share with the audience. Discussion with experts at the WWTmod seminar shall facilitate identifying critical knowledge gaps in current WWTP influent disturbance models. Finally, the outcome of these discussions will be used to define specific tasks that should be tackled in the near future to achieve more general acceptance and use of WWTP influent generators.

Global sensitivity analysis applied to drying models for one or a population of granules

The development of mechanistic models for pharmaceutical processes is of increasing importance due to a noticeable shift toward continuous production in the industry. Sensitivity analysis is a powerful tool during the model building process. A global sensitivity analysis (GSA), exploring sensitivity in a broad parameter space, is performed to detect the most sensitive factors in two models, that is, one for drying of a single granule and one for the drying of a population of granules [using population balance model (PBM)], which was extended by including the gas velocity as extra input compared to our earlier work. beta(2) was found to be the most important factor for the single particle model which is useful information when performing model calibration. For the PBM-model, the granule radius and gas temperature were found to be most sensitive. The former indicates that granulator performance impacts drying behavior, the latter is informative with respect to the variables that primarily need to be controlled during continuous operation. In addition, several GSA techniques are analyzed and compared with respect to the correct conclusion and computational load. (c) 2014 American Institute of Chemical Engineers AIChE J, 60: 1700-1717, 2014
Main Research Area: Technical/natural sciences

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- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.11 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
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.309 SNIP 1.64
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.297 SNIP 1.654
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 1.694 SNIP 1.578
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 1.749 SNIP 1.725
- Web of Science (2002): Indexed yes
- Scopus rating (2001): SJR 2.16 SNIP 2.077
- Web of Science (2001): Indexed yes
Hazard identification by extended multilevel flow modelling with function roles.

HAZOP studies are widely accepted in chemical and petroleum industries as the method for conducting process hazard analysis related to design, maintenance and operation of the systems. In this paper, a HAZOP reasoning method based on function-oriented modelling, multilevel flow modelling (MFM) is extended with function roles to complete HAZOP studies in principle. A graphical MFM editor, which is combined with the reasoning engine (MFM Workbench) developed by DTU is applied to automate HAZOP studies. The method is proposed to support the 'brain-storming' sessions in traditional HAZOP analysis. As a case study, the extended MFM-based HAZOP methodology is applied to an offshore three-phase separation process. The results show that the cause-consequence analysis in MFM can infer the cause and effect of a deviation used in HAZOP and used to fill HAZOP worksheet. This paper is the first paper discussing and demonstrating the potential of the roles concept in MFM to supplement the completeness of HAZOP analysis in theory.

HIDiC - Design, Sensitivity and Graphical Representation

We have explored the applicability of recent design methods based on H-xy diagrams for the HIDiC [i,ii] also for non-ideal and azeotropic systems. When applied together with sensitivity analysis and verification through rigorous simulations based on a newly developed and detailed HIDiC model, these concepts widen the scope of HIDiC design of a larger range of industrially relevant separations.
HIIDiC - Design, Sensitivity and Graphical Representation
The internally heat integrated distillation column (HIIDiC) is a potential replacement for the conventional distillation column for certain applications, offering reduced utility consumption of separation in more complex equipment. In addition, the conceptual design of the HIIDiC is significantly more difficult and classical short-cut methods such as that of McCabe-Thiele are not eligible. This work provides an application of a proposed algorithm for systematically generating feasible HIIDiC designs for the separation of isopropanol/water (IPA/W).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark, Université de Toulouse, Harper-Vedel
Authors: Meyer, K. (Ekstern), Ianniciello, L. (Ekstern), Nielsen, J. E. (Ekstern), Bisgaard, T. (Intern), Huusom, J. K. (Intern), Abildskov, J. (Intern)
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Hybrid Distillation Schemes: Design, Analysis & Application

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Babi, D. K. (Intern), Gani, R. (Intern)
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Identification and use of an alkane transporter plug-in for application in biocatalysis and whole-cell biosensing of alkanes
Effective application of whole-cell devices in synthetic biology and biocatalysis will always require consideration of the uptake of molecules of interest into the cell. Here we demonstrate that the AlkL protein from Pseudomonas putida GPo1 is an alkane import protein capable of industrially relevant rates of uptake of C7-C16 n-alkanes. Without alkL expression, native E.coli n-alkane uptake was the rate-limiting step in both the whole-cell bioconversion of C7-C16 n-alkanes and in the activation of a whole-cell alkane biosensor by C10 and C11 alkanes. By coexpression of alkL as a transporter plug-in, specific yields improved by up to 100-fold for biodissolution of C12 alkanes to fatty alcohols and acids. The alkL protein was shown to be toxic to the host when overexpressed but when expressed from a vector capable of controlled induction, yields of alkane oxidation were improved a further 10-fold (8 g/L and 1.7 g/g of total oxidized products). Further testing of activity on n-octane with the controlled expression vector revealed the highest reported rates of 120 μmol/min/g and 1 g/L/h total oxidized products. This is the first time AlkL has been shown to directly facilitate enhanced uptake of C10-C16 alkanes and represents the highest reported gain in product yields resulting from its use.
Identification and Use of an Alkane

Identification of Critical Parameters in Liquid Enzyme-Catalyzed Biodiesel Production

Callera™ Trans L, a liquid formulation of Thermomyces lanuginosus lipase, has recently shown great promise as a cost-efficient catalyst for methanolysis of triglyceride substrates, specifically in the BioFAME process. However, identifying the right combination of temperature and concentrations of catalyst, water and methanol to realize the full potential of the reaction system has remained a challenge. This study presents an investigation of the impact of temperature, enzyme and water concentration on the reaction, as well as the effect of methanol feed rate for the conversion of rapeseed oil in a fed-batch reaction system. It was observed that the reaction can be divided into two distinct parts. The first part of the reaction, during which primarily tri- and diglycerides are converted, proceeded at a high rate and thus required a high rate of methanol supply. The second part of the reaction, where the remaining di- and monoglycerides are converted, proceeded...
at a much lower rate. Consequently, it is necessary to reduce the methanol feed rate during the latter part of the reaction to avoid inhibition or even inactivation of the enzyme. Since the second part of the reaction occupied most of the 24-h reaction time, it was concluded that this is the part of the process where further development efforts should be targeted. This point was demonstrated by partially substituting the catalyst with a lipase with a different specificity, which enhanced the performance during the second phase of the reaction.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark, Novozymes A/S
Authors: Nordblad, M. (Intern), Silva, V. T. L. (Ekstern), Nielsen, P. M. (Ekstern), Woodley, J. M. (Intern)
Pages: 2446–2453
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 4.14 SJR 1.411 SNIP 1.163
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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
Impact on Model Uncertainty of Diabatization in Distillation Columns

This work provides uncertainty and sensitivity analysis of design of conventional and heat integrated distillation columns using Monte Carlo simulations. Selected uncertain parameters are relative volatility, heat of vaporization, the overall heat transfer coefficient, tray hold-up, and adiabatic index. Error propagation of uncertain parameters to second-law efficiency, the operation expenditures, the capital expenditures, and the dominant time constant for separations of benzene-toluene and benzene-flourobenzene are investigated. Conclusions favoring the HIDiC over the CDiC w.r.t. operation expenditures in the benzene-toluene separation can not made within 95% confidence. The sensitivity of overall heat transfer coefficient decreases on all indicators as the separation becomes more difficult.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Bisgaard, T. (Intern), Huusom, J. K. (Intern), Abildskov, J. (Intern)
Publication date: 2014
Implementation of a Process Intensification Approach in the Production of an API Intermediate

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CHEC Research Centre, The Danish Polymer Centre, H. Lundbeck A/S, Technical University of Denmark
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences

Improving Prediction Capability of Modelling Framework for Biphasic Reaction System

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Anantpinijwatna, A. (Intern), Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Publication date: 2014
Main Research Area: Technical/natural sciences

Incident at university research facility - melt down of gas chromatograph evaporation block and failure of a passive safety barrier.

Two incidents are described highlighting the importance of process hazard analysis in university laboratories. In the first incident, an online gas chromatograph (GC) was being developed. A complete meltdown of the heating blog was experienced during testing because the PC had failed to turn off the heating of the evaporation circuit. There had been no design review of the GC, nor any code review of the software controlling the GC. Neither had there been any management of change review for the introduction of the GC in the pilot plant environment, and so the GC had been introduced without any additional safety interlocks. In the second incident, a PhD student was pumping a mixture of water, methanol and isopropanol from an underground tank to the sewer while diluting it with water. The water lock of the sewer line was broken, and the mixture drained into the basement of the building instead of the sewer. From there, vapours spread to nearby facilities including an office building with many office workers and other laboratory facilities. A hazard analysis would have indicated the need to keep basement doors closed and only opened on an as-needed basis. If a hydrocarbon detector had been present in the basement it would have quickly alerted staff towards the source of the problem.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Safepark Consultancy
Authors: Jensen, N. (Ekstern), Jergensen, S. B. (Intern)
Pages: 17-19
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Loss Prevention Bulletin
Issue number: 238
ISSN (Print): 0260-9576
Ratings:
ISI indexed (2013): ISI indexed no
Incident at university research facility - pressure testing of gas hydrate cell
A master student designed a cell for observing the development of gas hydrates as conditions in the cell were changed. The supervisor asked for a pressure test of the cell before the experiments started. The student chose to perform the pressure test using compressed air and this resulted in one of the two windows on the cell breaking during the pressure test, resulting in glass fragments showering the laboratory. Luckily no one was hurt. Following this, and other incidents, the university implemented a requirement for a process hazard analysis (PHA) of any new or modified experimental set-ups in the department. This has been successfully used for a number of years to increase student appreciation of process safety in the laboratories and the safety of their workplace.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Safepark Consultancy
Authors: Jensen, N. (Ekstern), Jørgensen, S. B. (Intern)
Pages: 15-16
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Loss Prevention Bulletin
Issue number: 238
ISSN (Print): 0260-9576

Industrial process water treatment and reuse: A framework for synthesis and design
Mathematical optimization has shown the potential to contribute to industrial water management, through the development of the solution methods needed for optimization-based design of wastewater treatment and reuse networks (also called water networks). Nevertheless, the application of this approach is still limited to motivating examples lacking the ability to handle problems with complexity of industrial relevance. To address this challenge, in this contribution, we focus on the integration of wastewater engineering concepts and models, together with optimization methods and solution algorithms. To this end, we propose a computer-aided framework for the design of water treatment and reuse networks. In the framework, optimization methods, problem analysis tools and wastewater engineering knowledge are integrated in a computer-aided environment, in order to facilitate the formulation and solution of the design problems with fair complexity representative of industrial applications. The framework is demonstrated through the solution of a case study dealing with the treatment and reuse of water effluent produced by an oil refinery. The problem is solved, and a win-win solution is identified, allowing a reduced water footprint, and the treatment costs are identified.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark, University of Maribor
Authors: Quaglia, A. (Intern), Pennati, A. (Ekstern), Bogataj, M. (Ekstern), Kravanja, Z. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 12
Pages: 5160–5171
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 53
Influence of selecting secondary settling tank sub-models on the calibration of WWTP models – A global sensitivity analysis using BSM2

This study investigates the sensitivity of wastewater treatment plant (WWTP) model performance to the selection of one-dimensional secondary settling tanks (1-D SST) models with first-order and second-order mathematical structures. We performed a global sensitivity analysis (GSA) on the benchmark simulation model No.2 with the input uncertainty associated to the biokinetic parameters in the activated sludge model No. 1 (ASM1), a fractionation parameter in the primary clarifier, and the settling parameters in the SST model. Based on the parameter sensitivity rankings obtained in this study, the settling parameters were found to be as influential as the biokinetic parameters on the uncertainty of WWTP model predictions, particularly for biogas production and treated water quality. However, the sensitivity measures were found to be dependent on the 1-D SST models selected. Accordingly, we suggest a different optimum parameter selection for the calibration of WWTP models when either of the 1-D SST models is used. Using first-order models, the calibration should give equal importance to the adjustment of the hindered settling and slow settling parameter values. The adjusted hindered settling parameters have, however, no physical meaning, and might additionally obtain unrealistic values. In contrast, using second-order SST models, the focus of calibration should be on providing measured values for the hindered settling parameters. This approach is in close agreement with the recommendations made in the Good Modelling Practice protocol on activated sludge modelling. Besides, based on the GSA results, adjusting the non-measurable slow settling parameter produces significantly less variance in the model outputs using the second-order model than using the first-order model.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center, Lund University
Authors: Ramin, E. (Intern), Flores Alsina, X. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Jeppsson, U. (Ekstern), Mikkelsen, P. S. (Intern), Plósz, B. G. (Intern)
Pages: 28-34
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Publication information
Journal: Chemical Engineering Journal
Volume: 241
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Ratings:
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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
Inhibition of Gas Hydrate Nucleation and Growth: Efficacy of an Antifreeze Protein from the Longhorn Beetle *Rhagium mordax*

Antifreeze proteins (AFPs) are characterized by their ability to protect organisms from subfreezing temperatures by preventing tiny ice crystals in solution from growing as the solution is cooled below its freezing temperature. This inhibition of ice growth is called antifreeze activity, and in particular, certain insect AFPs show very high antifreeze activity. Recent studies have shown AFPs to be promising candidates as green and environmentally benign inhibitors for gas hydrate formation. Here we show that an insect antifreeze protein from the longhorn beetle, *Rhagium mordax* (RmAFP1), the most potent protein yet found for freezing inhibition, can inhibit methane hydrates as effectively as the synthetic polymeric inhibitor polyvinylpyrrolidone (PVP). In high pressure rocking cell experiments, onset hydrate nucleation temperatures and growth profiles showed repeatable results. RmAFP1 clearly showed inhibition of hydrates compared to amino acids (l-valine and l-threonine) and the protein bovine serum albumin (BSA). This indicates that proteins or amino acids do not generally inhibit hydrate formation. The promising performance of RmAFP1 as a new green kinetic hydrate inhibitor could further the development and increased production of green hydrate inhibitors.

**General information**

**State:** Published  
**Organisations:** Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS, Technical University of Denmark, University of Stavanger, Roskilde Universitet  
**Authors:** Perfeldt, C. M. (Ekstern), Chua, P. C. (Ekstern), Daraboina, N. (Intern), Friis, D. (Ekstern), Kristiansen, E. (Ekstern), Ramløv, H. (Ekstern), Woodley, J. (Intern), Keilland, M. A. (Ekstern), von Solms, N. (Intern)  
**Number of pages:** 7  
**Pages:** 3666-3672  
**Publication date:** 2014  
**Main Research Area:** Technical/natural sciences

**Publication Information**

**Journal:** Energy and Fuels  
**Volume:** 28  
**Issue number:** 6  
**ISSN (Print):** 0887-0624  
**Ratings:**  
BFI (2018): BFI-level 2  
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

Key developments of instrumentation, control and automation (ICA) applications in wastewater systems during the past 40 years are highlighted in this paper. From the first ICA conference in 1973 through to today there has been a tremendous increase in the understanding of the processes, instrumentation, computer systems and control theory. However, many developments have not been addressed here, such as sewer control, drinking water treatment and water distribution control. It is hoped that this review can stimulate new attempts to more effectively apply control and automation in water systems in the coming years.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University, Uppsala University, University of Girona, Primodal Inc., Grundfos A/S, Pusan National University, inCTRL Solutions Inc., INRA Institut National de La Recherche Agronomique, Dynamita, Universite Laval, Instituto de Ingenieria, University of Queensland, Swedish Environmental Research Institute
Pages: 1373-1385
Publication date: 2014
Integration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process design

The sustainable future of the world challenges engineers to develop chemical process designs that are not only technically and economically feasible but also environmentally friendly. Life cycle assessment (LCA) is a tool for identifying and quantifying environmental impacts of the chemical product and/or the process that makes it. It can be used in conjunction with process simulation and economic analysis tools to evaluate the design of any existing and/or new chemical-biochemical process and to propose improvement options in order to arrive at the best design among various alternatives. Although there are several commercial LCA tools, there is still a need for a simple LCA software that can be integrated with process design tools. In this paper, a new LCA software, LCSoft, is developed for evaluation of chemical, petrochemical, and biochemical processes with options for integration with other process design tools such as sustainable design (SustainPro), economic analysis (ECON) and process simulation. The software framework contains four main tools: Tool-I is for life cycle inventory (LCI) knowledge management that enables easy maintenance and future expansion of the LCI database; Tool-2 is for estimation of environmental impact characterization factors using group contribution (+) method (GC(+)) in order to calculate environmental impacts for a wide range of chemicals; Tool-3 performs LCA calculations based on a library of models; and, Tool-4 provides interfaces for integration with other tools. To test the software, a bioethanol production process using cassava rhizome is employed as a case study. Results from LCSoft highlight the estimated environmental performance in terms of various aspects such as carbon footprint, resource and energy consumptions, and various environmental impacts. (C) 2014 Elsevier Ltd. All rights reserved.
Introducing an In Situ Capping Strategy in Systems Biocatalysis To Access 6-Aminohexanoic acid

The combination of two cofactor self-sufficient biocatalytic cascade modules allowed the successful transformation of cyclohexanol into the nylon-6 monomer 6-aminohexanoic acid at the expense of only oxygen and ammonia. A hitherto unprecedented carboxylic acid capping strategy was introduced to minimize the formation of the deadend intermediate 6-hydroxyhexanoic acid. For this purpose, the precursor e-caprolactone was converted in aqueous medium in the presence of methanol into the corresponding methyl ester instead of the acid. Hence, it was shown for the first time that esterases—specifically horse liver esterase—can perform the selective ring-opening of e-caprolactone with a clear preference for methanol over water as the nucleophile.
Introducing an In Situ Capping Strategy in Systems Biocatalysis To Access 6-Aminohexanoic acid

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Ionic-Liquid Based Separation of Azeotropic Mixtures

methodology for the screening of ionic liquids (ILs) as entrainers for ILs-based separation processes in binary aqueous azeotropic systems (e.g., water + ethanol and water + isopropanol) is presented. Ionic liquids as entrainers were first screened based on a combination of criteria such as stability, toxicity, and environmental impacts of the ILs. A Hildebrand solubility parameter group contribution model for ILs is highlighted to screen the miscibility of the ILs with the target solute component which was considered as a key target property to further screen the candidates from the previous step. The best candidates for aqueous systems were selected for final evaluation as follows: 1-ethyl-3-methylimidazolium ethylsulfate [C2MIM][EtSO4], 1-ethyl-3-methylimidazolium acetate [C2MIM][Ac], 1-ethyl-3-methylimidazolium dicyanamide
For the final evaluation, the best candidates for aqueous systems were used as entrainers, and then the vapor-liquid equilibrium (VLE) of the ternary systems containing ILs was predicted by the Non Random Two Liquids (NRTL) model to confirm the breaking of the azeotrope. Based on minimum concentration of the ILs required to break the given azeotrope, the best ILs as entrainers for water + ethanol and water + isopropanol azeotropic mixtures were [C1MIM][DMP] and [C2MIM][N(CN)2], respectively.

**Kinetic study on the enzymatic esterification of octanoic acid and hexanol by immobilized Candida antarctica lipase B**

This study investigates reaction kinetics of the esterification of octanoic acid and hexanol into hexyloctanoate, catalyzed by an immobilized Candida antarctica lipase (Novozym®435). The product is considered natural and used as a fresh vegetable and fruity flavour additive in food, cosmetic and pharmaceutical products. The reaction is performed in n-decane as the solvent, to improve enzyme stability and to increase the reaction yield. The influence of substrate concentration on hexyl octanoate synthesis is investigated over a wide range up to 2 M. The observed bi-substrate inhibition pattern follows a Ping-Pong bi-bi mechanism with dead-end inhibition by both substrates and, based on the proposed model, the kinetic constants of the esterification reaction are estimated. These parameters are verified to be intrinsic – neither external nor internal mass transfer resistances are significant for the examined reaction system – and are essential to extend analysis to a large-scale process and for a wide range of operating conditions. The progress of the reaction is also observed and the kinetic model is validated by fitting experimental progress curves with two different concentrations of biocatalyst. Effects of biphasicity of the reaction system, inhibition by the ester produced and the influence of the reverse reaction have been also evaluated.© 2014 Elsevier B.V. All rights reserved.
Managing the Complexity in Chemical Product Engineering

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern)
Publication date: 2014
Event: Abstract from INVITED SEMINAR 2014, Chicago, United States.
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 102382550
Publication: Research - peer-review › Journal article – Annual report year: 2014

Original language: English
Kinetics, Hexyl octanoate, Lipase Novozym, Ping-Pong bi-bi, Enzymatic esterification
DOIs: 10.1016/j.molcatb.2014.09.011
Source: PublicationPreSubmission
Source-ID: 103527888
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014
Measurement of VLE data for binary lipids systems
Consistent physical and thermodynamic properties of pure components and their mixtures are important for process
design, simulation, and optimization as well as design of chemical based products. In the case of lipids, our previous
works[1-3] have indicated a lack of experimental data for pure components and also for their mixtures. To contribute in this
area, experimental data were obtained using the Differential Scanning Calorimetry (DSC) technique for isobaric vapor-
liquid equilibrium (VLE) of two binary mixtures at two different pressures (1.2 and 2.5 KPa): system 1 [monoacylglycerol
(monocaprylin) + fatty acid (palmitic acid)] and system 2 [monoacylglycerol (monocaprylin) + fatty ester (methyl stearate)].
System 1 is relevant in the purification steps of the deodorizer distillates while system 2 is relevant in the purification steps
of biodiesel and bioglycerin. A non-ideal behavior is revealed for both systems at the two different pressures, with
azeotrope behavior observed and confirmed but the relative volatility analysis. Available thermodynamic consistency tests
for TPx data were applied before performing parameter regressions for Wilson NRTL, UNIQUAC and original UNIFAC
models. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of
predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC
model. A new group for original UNIFAC model is created aiming to improve the representation of the experimental data
by this predictive model.

Measuring and modelling of the combined thermodynamic promoting effect of tetrahydrofuran and cyclopentane on carbon
dioxide hydrates
This work documents both experimental data, and by thermodynamic modelling, the synergistic effect occurring in
promoted carbon dioxide hydrate systems at the simultaneous presence of tetrahydrofuran and
cyclopentane. Cyclopentane has previously been considered a reference among gas hydrate promoters due to its
significant pressure reducing effect in hydrate forming systems such as those related to carbon dioxide capture. The
present work shows that hydrate dissociation pressures may be lowered by up to 22% compared to those of the
cyclopentane promoted carbon dioxide hydrate system by addition of tetrahydrofuran to the aqueous phase. It is shown
experimentally that addition of approximately 5 mol% tetrahydrofuran to the aqueous phase of the cyclopentane promoted
system, reduces hydrate formation pressures by approximately 20% compared to those of the cyclopentane promoted
system at similar temperatures. A thermodynamic model, based on the van der Waals–Platteeuw model and the cubic-
plus-association equation of state is applied to model the mixed promoter system. The model accurately predicts the data
measured in this work. Furthermore, the model explains the synergistic effect by the fact that tetrahydrofuran displaces
cyclopentane from the large cavities of the sII hydrate structure. The most pronounced synergistic effect (largest pressure
reduction) is predicted at scenarios, where approximately half of the cyclopentane in the hydrate phase has been
substituted with tetrahydrofuran. The model predicts the maximum pressure reduction compared to the cyclopentane
promoted system to be approximately 22%. This happens at tetrahydrofuran concentrations of approximately 2.8–3.1
mol% in the aqueous phase, depending on the system temperature.
Mechanistic Modelling of Biodiesel Production using a Liquid Lipase Formulation

In this article, a kinetic model for the enzymatic transesterification of rapeseed oil with methanol using Callera™ Trans L (a liquid formulation of a modified Thermomyces lanuginosus lipase) was developed from first principles. We base the model formulation on a Ping-Pong Bi-Bi mechanism. Methanol inhibition, along with the interfacial and bulk concentrations of the enzyme was also modeled. The model was developed to describe the effect of different oil compositions, as well as different water, enzyme, and methanol concentrations, which are relevant conditions needed for process evaluation, with respect to the industrial production of biodiesel. The developed kinetic model, coupled with a mass balance of the system, was fitted to and validated on experimental results for the fed-batch transesterification of rapeseed oil. The confidence intervals of the parameter estimates, along with the identifiability of the model parameters were presented. The predictive capability of the model was tested for a case using 0.5% (wt. Enzyme/wt. Oil), 0.5% (wt. Water /wt. Oil) and feeding 1.5 times the stoichiometric amount of methanol in total over 24 h. For this case, an optimized methanol feeding profile that constrains the amount of methanol in the reactor was computed and the predictions experimentally validated. Monte-Carlo simulations were then used to characterize the effect of the parameter uncertainty on the model outputs, giving a biodiesel yield, based on the mass of oil, of 90.8 ± 0.55 mass %. © 2014 American Institute of Chemical Engineers

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
Authors: Price, J. A. (Intern), Hofmann, B. (Ekstern), Silva, V. T. L. (Ekstern), Nordblad, M. (Intern), Woodley, J. M. (Intern), Huusom, J. K. (Intern)
Number of pages: 14
Pages: 1277–1290
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Biotechnology Progress
Volume: 30
Issue number: 6
ISSN (Print): 8756-7938
Ratings:
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 2.12 SJR 0.668 SNIP 0.762
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.727 SNIP 0.825 CiteScore 2.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.808 SNIP 0.931 CiteScore 2.2
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.764 SNIP 0.847 CiteScore 2.16
Mechanistic Modelling Of Enzymatic Biodiesel Production For Fed Batch Control

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Price, J. A. (Intern), Nordblad, M. (Intern), Woodley, J. (Intern), Huusom, J. K. (Intern)
Number of pages: 1
Publication date: 2014
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9531
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013
Mixing and transport during pharmaceutical twin-screw wet granulation: Experimental analysis via chemical imaging

Twin-screw granulation is a promising continuous alternative for traditional batch high shear wet granulation (HSWG). The extent of HSWG in a twin screw granulator (TSG) is greatly governed by the residence time of the granulation materials in the TSG and degree of mixing. In order to determine the residence time distribution (RTD) and mixing in TSG, mostly visual observation and particle tracking methods are used, which are either inaccurate and difficult for short RTD, or provide an RTD only for a finite number of preferential tracer paths. In this study, near infrared chemical imaging, which is more accurate and provides a complete RTD, was used. The impact of changes in material throughput (10–17 kg/h), screw speed (500–900 rpm), number of kneading discs (2–12) and stagger angle (30–90 °) on the RTD and axial mixing of the material was characterised. The experimental RTD curves were used to calculate the mean residence time, mean centred variance and the Pécelt number to determine the axial mixing and predominance of convective over dispersive transport. The results showed that screw speed is the most influential parameter in terms of RTD and axial mixing in the TSG and established a significant interaction between screw design parameters (number and stagger angle of kneading discs) and the process parameters (material throughput and number of kneading discs). The results of the study will allow the development and validation of a transport model capable of predicting the RTD and macro- mixing in the TSG. These can later be coupled with a population balance model in order to predict granulation yields in a TSG more accurately.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Ghent University, VTT - Technical Research Centre of Finland
Pages: 279-289
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Main Research Area: Technical/natural sciences

Publication information
Journal: European Journal of Pharmaceutics and Biopharmaceutics
Volume: 87
Issue number: 2
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Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.49 SJR 1.366 SNIP 1.409
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.414 SNIP 1.496 CiteScore 4.37
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.469 SNIP 1.586 CiteScore 4.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.558 SNIP 1.706 CiteScore 4.64
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.976 SNIP 1.933 CiteScore 5.15
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.794 SNIP 1.887 CiteScore 4.77
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.948 SNIP 1.933
BFI (2009): BFI-level 2
Modeling and optimizing oxygen transfer in small scale reactors using computational fluid dynamics

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Larsson, H. (Intern), Gernaey, K. (Intern), Krühne, U. (Intern)
Number of pages: 1
Publication date: 2014
Main Research Area: Technical/natural sciences
Electronic versions:
IMRET_hilde_final.pdf
Source: PublicationPreSubmission
Source-ID: 116514966
Publication: Research - peer-review › Poster – Annual report year: 2015

Modelling across bioreactor scales: methods, challenges and limitations
Scale-up and scale-down of bioreactors are very important in industrial biotechnology, especially with the currently available knowledge on the occurrence of gradients in industrial-scale bioreactors. Moreover, it becomes increasingly appealing to model such industrial scale systems, considering that it is challenging and expensive to acquire experimental data of good quality that can be used for characterizing gradients occurring inside a large industrial scale bioreactor. But which model building methods are available? And how can one ensure that the parameters in such a model are properly estimated? And what are the limitations of different types of models? This paper will provide examples of models that have been published in the literature for use across bioreactor scales, including computational fluid dynamics (CFD) and population balance models. Furthermore, the importance of good modeling practice will be highlighted as well.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gernaey, K. (Intern)
Publication date: 2014
Main Research Area: Technical/natural sciences
Electronic versions:

Bibliographical note
INVITED KEYNOTE LECTURE.
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Source-ID: 103604783
Modelling and operation of reactors for enzymatic biodiesel production

In developing sustainable industrial processes, biochemical engineering, as a part of a broader field of chemical engineering is becoming an increasingly important as a tool in the chemical engineers toolbox. Its application is driven by consumer demand for new products and by industry wishing to increase profits while reducing operating cost, as well as meeting government and regulatory pressures for processes to be environmentally friendly and sustainable. Current applications of biocatalysts, more specifically, enzymes for large scale bulk production of chemicals have been successfully applied to the production of high fructose corn syrup, upgrading of fats and oils and biodiesel production to name a few. Despite these examples of industrial enzymatic applications, it is still not "clear cut" how to implement biocatalyst in industry and how best to optimize the processes. This is because the processing strategy is usually different to most traditional catalytic processes. In nature, enzymes operate at much lower substrate and product concentrations compared to most industrial chemical processes. What this means is that the natural conditions for biocatalysts are normally much different from conventional process-relevant conditions. Also, the optimal process conditions can vary greatly from one biocatalyst to the next. Hence, to maximize product yields and reactor productivity then the type of reactor operation and downstream processing need to be able to address the aforementioned issues. One way to achieve this is through process modelling to help focus the experimental work needed for process understanding and to support further process development and optimization of the process.

To address how the reactors should be operated; a strategy using mechanistic modelling by combining the biological aspects of the enzyme with reaction/reactor engineering is performed. This strategy is applied to a case study of biodiesel production catalysed by a liquid enzyme formulation. The use of enzymes for biodiesel production is still in its infancy with non-optimized process designs. Furthermore is it unclear how the process should be operated to ensure optimal economics given the relatively high cost of the enzyme and the low value of the products.

General information
State: Published
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Modelling and optimization of C5 and C6 fermentation: focus on pH impact and Inhibitors effect

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
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Modelling N2O dynamics in the engineered N cycle: Evaluation of alternate model structures

Research on nitrous oxide (N2O) formation in engineered wastewater systems has experienced an exponential development in the recent years due to the important environmental impact of this greenhouse gas. These efforts have crystallized in a large number of publications that aim to identify the importance of the main microbial processes responsible for its production and consumption. The conceptualization of these pathways in mathematical models has the potential to become a key tool to increase our understanding on the complex interrelationships within these ecosystems and develop strategies to minimize the carbon footprint of wastewater treatment plants. The present contribution aims to summarize the recent developments in this field and makes use of standard identifiability measures to show how the choice of experimental protocols and model structures can potentially impact their calibration.

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Modelling of cyclopentane promoted gas hydrate systems for carbon dioxide capture processes

A thermodynamic model based on the Cubic-Plus-Association equation of state and the van der Waals-Platteeuw hydrate model is applied to perform a thermodynamic evaluation of gas hydrate forming systems relevant for post-combustion carbon dioxide capture. A modelling study of both fluid phase behaviour and hydrate phase behaviour is presented. Cycloalkanes ranging from cyclopropane to cyclohexane, represents a challenge for CPA, both in the description of the pure component densities and for liquid-liquid equilibrium (LLE) in the binary systems with water. It is concluded that an insufficient amount of reliable LLE data exist for the binary system of water and cyclopentane. Additional water-in-oil data in particular are desired for this system. An unpromoted hydrate-based capture process, operating isothermally at a temperature of 280 K is simulated. The minimum pressure requirement of the first stage is estimated to be 24.9 MPa. Applying three consecutive hydrate formation/dissociation stages (three-stage capture process), a carbon dioxide-rich product (97 mol%) may be delivered at a temperature of 280 K and a pressure of 3.65 MPa. A second capture process, where cyclopentane is incorporated as a thermodynamic hydrate promoter is simulated. At the presence of cyclopentane the minimum pressure requirement of the first stage (operating at 285 K) is lowered to 1.04 MPa. The vapour phases in the cyclopentane promoted process contains several mole percent cyclopentane at hydrate equilibrium conditions. At temperatures below 284 K, the entire cyclopentane bulk phase evaporates completely at hydrate forming conditions (pressures below 0.55 MPa). The present study suggests the hydrate-based separation technology to be unsuitable for the specific case of post-combustion carbon dioxide capture from power station flue gases, where operating pressures should preferably remain close to atmospheric. Even though the hydrate structure becomes available at low pressure conditions (by use of thermodynamic promoters), carbon dioxide may not necessarily enter the solid phase in significant amounts. © 2014 Elsevier B.V.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, CAPEC-PROCESS
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Main Research Area: Technical/natural sciences

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Modelling of tetrahydrofuran promoted gas hydrate systems for carbon dioxide capture processes

A thermodynamic study of a novel gas hydrate based CO2 capture process is presented. Model predicts this process unsuitable for CO2 capture from power station flue gases. A thermodynamic modelling study of both fluid phase behaviour and hydrate phase behaviour is presented for the quaternary system of water, tetrahydrofuran, carbon dioxide and nitrogen. The applied model incorporates the Cubic-Plus-Association (CPA) equation of state for the fluid phase description and the van der Waals-Platteeuw hydrate model for the solid (hydrate) phase. Six binary pairs are studied for their fluid phase behaviour. CPA descriptions are adjusted when needed by correlation of binary parameters in the applied mixing- and combining rules. Kihara cell potential parameters in the hydrate model are regressed for the three hydrate formers, tetrahydrofuran, carbon dioxide and nitrogen. The developed model provides highly accurate descriptions of both fluid- and hydrate phase equilibria in the studied system and its subsystems. The developed model is applied to simulate two simplified, gas hydrate-based processes for post-combustion carbon dioxide capture from power station flue gases. The first process, an unpromoted hydrate process, operates isothermally at a temperature of 280. K. Applying three consecutive hydrate formation/dissociation stages (three-stage capture process), a carbon dioxide-rich product (97. mol%) is finally delivered at a temperature of 280. K and a pressure of 3.65. MPa. The minimum pressure requirement of the first stage is estimated to be 24.9. MPa, corresponding to the incipient hydrate dissociation pressure at 280. K for the considered flue gas. A second simulated carbon dioxide capture process uses tetrahydrofuran as a thermodynamic promoter to reduce the pressure requirements. By doing so the minimum pressure requirement of the first capture stage is lowered to 0.41. MPa. Selectivity towards carbon dioxide in the hydrate phase is however lower than in the unpromoted process. Therefore the tetrahydrofuran promoted capture process needs four consecutive hydrate formation/dissociation stages to produce a 96. mol% carbon dioxide-rich product stream. This stream is delivered at 280. K and a pressure of 0.17. MPa. The present modelling study suggests several drawbacks of using tetrahydrofuran as a thermodynamic hydrate promoter, when applied in low-pressure, hydrate-based gas separation processes. Due to the high volatility of this compound, the promoter readily transfers to the vapour phase. Furthermore, tetrahydrofuran lowers the selectivity towards carbon dioxide, and the gas uptake in general, in the hydrate phase compared to the unpromoted system. © 2014 Elsevier B.V.
Modelling the occurrence, transport and fate of pharmaceuticals in wastewater systems

This paper demonstrates how occurrence, transport and fate of pharmaceuticals at trace levels can be assessed when modelling wastewater treatment systems using two case studies. Firstly, two approaches based on: 1) phenomenology; and, 2) Markov Chains, are developed to describe the dynamics of pharmaceuticals with or without clear administration patterns. Additional simulations also show that sewer conditions might have an important effect on the behaviour of the generated compounds and their metabolites. The results demonstrate that different operating conditions in wastewater treatment plants can have opposite effects on the studied pharmaceuticals, especially when they present co-metabolic or inhibitory behaviour in the presence of biodegradable substrate. Finally, the paper ends with: i) a critical discussion of the presented results; ii) a thorough analysis of the limitations of the proposed approach; and, iii) future pathways to improve the overall modelling of micropollutants.
Moisture and drug solid-state monitoring during a continuous drying process using empirical and mass balance models

Classically, the end point detection during fluid bed drying has been performed using indirect parameters, such as the product temperature or the humidity of the outlet drying air. This paper aims at comparing those classic methods to both in-line moisture and solid-state determination by means of Process Analytical Technology (PAT) tools (Raman and NIR spectroscopy) and a mass balance approach. The six-segmented fluid bed drying system being part of a fully continuous from-powder-to-tablet production line (ConsiGma™-25) was used for this study. A theophylline:lactose:PVP (30:67.5:2.5) blend was chosen as model formulation. For the development of the NIR-based moisture determination model, 15 calibration experiments in the fluid bed dryer were performed. Six test experiments were conducted afterwards, and the product was monitored in-line with NIR and Raman spectroscopy during drying. The results (drying endpoint and residual moisture) obtained via the NIR-based moisture determination model, the classical approach by means of indirect parameters and the mass balance model were then compared. Our conclusion is that the PAT-based method is most suited for use in a production set-up. Secondly, the different size fractions of the dried granules obtained during different experiments (fines, yield and oversized granules) were compared separately, revealing differences in both solid state of theophylline and moisture content between the different granule size fractions.

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Scopus rating (2012): SJR 1.976 SNIP 1.933 CiteScore 5.15
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Monitoring and modelling of a continuous from-powder-to-tablet process line

The intention to shift from batch to continuous production processes within the pharmaceutical industry enhances the need to monitor and control the process in-line and real-time to continuously guarantee the end-product quality. Mass and energy balances have been successfully applied to a drying process which is part of a continuous from-powder-to-tablet manufacturing line to calculate the residual moisture content of granules leaving the drying unit on the basis of continuously generated data from univariate sensors. Next to monitoring, the application of continuous processes demands also real-time adjustment of critical input variables to ensure that the process stays within the Design Space. Mechanistic models are very useful for this purpose as, once validated, several tools can be applied to gain further process knowledge, for example uncertainty and sensitivity analysis. In addition, several scenarios can be simulated, thus reducing the need to collect time-consuming, and often costly, experimental data.

General information

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Multi-dimensional population balance models of crystallization processes

A generic and model-based framework for batch cooling crystallization operations has been extended to incorporate continuous and fed-batch processes. Modules for the framework have been developed, including a module for reactions, allowing the study of reactive crystallization within the framework. A kinetic model library together with an ontology for knowledge representation has been developed, in which kinetic models and relations from the literature are stored along with the references and data. The model library connects to the generic modelling framework as well, as models can be retrieved, analyzed, used for simulation and stored again. The model library facilitates comparison of expressions for kinetic phenomena and is tightly integrated with the model analysis tools of the framework. Through the framework, a model for a crystallization operation may be systematically generated and parameters for the simulation can be found in the database. A procedure for parameter estimation has been illustrated based on experimental work. The identifiability of the models has been discussed in relation to parameter estimation using sensitivity analysis. Some important identifiability issues have been investigated using the model structure to simulate perfect data and data with white noise added to it. It is found that the kinetic models may not be reliably estimated from the concentration profile using the parameter estimation procedure for both perfect and noisy data. The framework has been applied to case studies involving inorganic and organic compounds, including an active pharmaceutical ingredient (paracetamol) crystallized from different solvents. The case studies have been used to demonstrate the versatility of the framework.

General information

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New Product Introduction in the Pharmaceutical Industry

Due to the limited time of the monopoly provided by patent protection that is used for recouping the R&D investment, pharmaceutical companies focus on keeping time-to-market for new products as short as possible. This process is however getting more uncertain, as the outcome of clinical trials is unknown and negotiations with authorities have become harder, making market introduction more difficult. This dissertation treats the new product introduction process in the pharmaceutical industry from an operations perspective. The overarching aim of this dissertation is to improve the planning methodology in this critical process. In an empirical study, the process is first analyzed in detail, leading to the identification of several gaps in the industry's current planning approaches. To support a set of key operational decisions towards market launch, a model is subsequently developed, considering uncertainty and several important industry characteristics. The model is used to gain several insights on the use of risk packaging and on keeping time-to-market short. As capacity in secondary pharmaceutical production is critical for product availability, a capacity planning model for a new drug delivery system is also developed. It captures the ramp-up phase in a better way, while considering inventory build up, plant validation and limited shelf life. The performance of several ramp-up functions is tested and insights into ramp-up management are presented. The dissertation is concluded with showing the new proposed planning structure, concluding in the preceding chapters and outlining future research possibilities.

On the Responses of Azeotropes to Pressure Variations

Systems with azeotropes cannot be separated by simple distillation since the vapor and liquid compositions are the same. Variation of the applied pressure can shift the azeotropic composition out of the range of purification of a single column or may allow pressure swing operation of two columns. Because of the sensitivity of column size to accurate estimates of the relative volatility, it is important to use reliable phase equilibrium thermodynamics when exploring the possibility of varying pressure to avoid an azeotrope. Based on an analysis of the pressure sensitivity of azeotropic compositions, we show examples of the impact of different modeling strategies for binary and multicomponent mixtures.
Operational Aspects of Continuous Pharmaceutical Production

Introduction of the Process Analytical Technology (PAT) Initiative, the Quality by Design (QbD) approach and the Continuous Improvement (CI) methodology/philosophy is considered as a huge milestone in the modern pharmaceutical industry. The above concepts, when applied to a pharmaceutical production process, should enable better designs of products and processes. Furthermore, easier process monitoring, control and automation are just some of the advantages that can be achieved as a consequence. Traditional production methods of Active Pharmaceutical Ingredients (APIs) are based on batch and semi-batch processes which include plenty of supportive actions defined as non-value added activities (NVAs) or simply waste. It is therefore desirable to implement a switch from batch based production to continuous manufacturing modes in order to minimize NVAs, as well as to enable easier satisfaction of the demands defined by the PAT Initiative. This approach could be considered as establishing a Lean Production System (LPS) which has usually supported with tools associated with Process Intensification (PI) and Process Optimization (PO). Development of continuous processes is often connected with many obstacles due to the very long reaction sequences, inhomogenous reaction mixtures, the presence of slurries.... It is therefore important to adapt the reaction conditions as much as possible to the desired production in continuous mode. Small-scale manufacturing could be supported with modern PI tools, such as microwave assisted organic synthesis (MAOS), ultrasounds, meso-scale flow chemistry and microprocess technology. Furthermore, development of chemical catalysts and enzymes enabled further acceleration of some chemical reactions that were known as very slow or impossible to be performed. The main goal of this work is to develop a PI strategy that would include different chemical and physical approaches with the main purpose to accelerate slow chemical reactions and adapt them to continuous manufacturing modes. Detailed insight into the PAT, QbD, CI and Lean Production System (LPS) is additionally provided in the introduction. The practical implementation of the PI strategy is covered with three different examples. The first example process is the dehydration of 9- Allyl-2-Chlorothioxanthene, 9-Ol ("N746-Butadienes") to the mixture of cis and trans 9H-thioxanthene, 2-chloro-9-(2-propenylidene) - (9CI) ("N746-Butadienes"). Both components are intermediate products in the synthesis of Zuclopenthixol – a product of H. Lundbeck A/S. Successful transfer from batch towards meso-flow chemistry is performed together with demonstration of the potential for in-/off-line process monitoring. The second example process is the anti-Markovnikov hydroamination between the "N746-Butadienes" and 1-(2-hydroxyethyl)piperazine (HEP) resulting into a mixture of cis/trans 4- [3 - 2 Chlorothioxanthene - 9 - ylidene]propyl] - 1 - pipерazineethanol (Clopenthixol). This chemical reaction is well-known as very slow and difficult to be accelerated by applying chemical catalysts. vi Some authors claim that hydroamination of unsaturated hydrocarbons is known as one of the “ten challenges for homogeneous catalysis”. Nevertheless, implementation of the PI strategy by using microwave irradiation resulted in significant improvements. The third example process includes the small-scale production of (2-Bromophenyl)(phenyl)sulfane. This important API intermediate is receiving significant attention in the pharmaceutical industry due to the fact that there are plenty of APIs which include C-S bonds in their chemical structure. The production of such compounds is based on Carbon-Sulfur cross coupling reactions, involving expensive chemical catalysts, chemical ligands, bases and unfriendly solvents. Implementation of the PI strategy with a significantly modified chemical pathway resulted in several benefits from an economic, environmental and manufacturing point of view. Considering the results achieved in the case studies, it can be concluded that successful implementation of
the PI strategy has been achieved while satisfying the PAT demands and implementing Lean Production System. Significant accelerations of often considered difficult chemical reactions have been achieved, and therefore it can be concluded that a successful transfer from batch towards continuous manufacturing has been achieved.

General information
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Oxidase-based biocatalytic processes
Biocatalytic processes are gaining significant focus in frontiers where they offer unique advantages (selectivity and mild operating conditions) over chemical catalysts. It is therefore not surprising that there have been many industrial biocatalytic processes implemented. Despite past successes, the implementation of a new biocatalytic process still presents some challenges (demands placed on the biocatalyst) in terms of the requirements to make a viable industrial process. In order for a biocatalytic process to be economically successful, it is necessary that certain set of target metrics (product titre, biocatalyst yield or space time yield and reaction yield) are achieved. Hence, the biocatalyst must be able to work at high substrate and product concentrations. Such constraints that arise from the biocatalyst are classified as biocatalyst-related limitations. In addition, other limitations can arise from the reaction species (substrate and product volatility for example) and the process (such as oxygen supply, ability to control pH) and are classified as reaction-related and process-related constraints respectively. Although the development of biocatalyst and process engineering tools offers a number of solutions to overcome the limitations, it is often complicated to identify the key limitation of the system that prevents economic scale-up. Hence, development of a systematic method for identifying the limitations during early-stage development of a biocatalytic process and potentially the order in which they need to be tackled would offer a valuable tool for process development. Biocatalytic oxidations are potentially of great value because of the selective chemistry that they offer, resulting in higher yields compared to those achievable through chemical catalysis. Oxidases are particularly interesting biocatalysts because they use a mild oxidant (oxygen) as a substrate as opposed to their chemical counterparts which use strong oxidants such as permanganates. A class of oxidases called monoamine oxidases has been used as the central case study for the thesis. The rationale for choosing this system is that it has been shown to exhibit the potential for resolution of racemic amines, and is capable of producing industrially interesting imines which are rather difficult to synthesize by chemical routes. An important aspect for biocatalytic reactions would be the implementation of monitoring and control systems that allow for rapid data collection to gain process knowledge. For oxidase-based biocatalysis, oxygen is consumed in stoichiometric amounts for the reaction. Therefore, oxygen sensors which can measure the oxygen concentration can be a valuable tool for monitoring the process. The thesis exemplifies the use of novel solvent-resistant oxygen sensors as supporting technology for oxidase-based reactions using a glucose oxidase reaction system as an example. Implementation of biocatalytic oxidation at scale still requires process knowledge which includes the limitations of the system and the knowledge about the potential solutions available to alleviate these limitations. This thesis presents a methodology for development of oxidase-based biocatalytic processes. Particularly important aspect of the methodology includes the use of optimisation tools where property prediction tools have been used to identify the potential limitations to the reaction system prior to experimentation. Such an analysis presents the opportunity to direct experimental work and therefore reduce the time and effort spent on process development, by eliminating unfeasible
routes. The example chosen for the development of the methodology was a specific monoamine oxidase-based syntheses for the production of a pharmaceutical intermediate. This particular reaction system was chosen because of the potential use of the product of the biocatalytic reaction as a pharmaceutical intermediate. However, there was little information on the reaction system in the literature for the use of this biocatalyst for the synthesis of chemicals. Therefore, early stage process understanding was required. The chapters of the thesis identify the potential limitations for the reaction system by systematic evaluation of the reaction system through the use of property prediction tools as well as experiments. The results obtained from the experiments are then used to identify the bottleneck for the implementation at scale. Furthermore, discussion of the limitations and the order in which they need to be tackled is presented.
MFM Model Editing Interface to facilitate the modelling process and MFM model analysis modules to run diagnosis and prognosis analyses based on developed models. New features of the MFM Suite also include making corresponding process diagram for the plant being modelled with MFM and linking the MFM model to its process components. The purpose of this report is to make a comprehensive demonstration of how to use the MFM Suite to develop MFM models and run causal reasoning for abnormal situations. This report will explain the capability of representing process and operational knowledge by using the MFM methodology, and demonstrate how the model combined with the MFM reasoning can be used to evaluate the plant state, identify the current situation and support operational decisions. The report will provide a detailed explanation of MFM concepts by modelling the primary side system of the Ringhals Westinghouse PWR and demonstrate the MFM reasoning for accident situation.

General information
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Organisations: Department of Electrical Engineering, Automation and Control, Center for Electric Power and Energy, Energy system operation and management, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, OECD Halden Reactor Project, Safepark Consultancy
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Pressure Control in Distillation Columns: A Model-Based Analysis
A comprehensive assessment of pressure control in distillation columns is presented, including the consequences for composition control and energy consumption. Two types of representative control structures are modeled, analyzed, and benchmarked. A detailed simulation test, based on a real industrial distillation column, is used to assess the differences between the two control structures and to demonstrate the benefits of pressure control in the operation. In the second part of the article, a thermodynamic analysis is carried out to establish the influence of pressure on relative volatility for (pseudo)binary mixtures. A simple criterion is found, based on the difference in the scaled heats of vaporization of the light and heavy compounds: A large difference indicates that relative volatility is sensitive to pressure changes, whereas no a priori conclusion can be made for small differences. Depending on the sensitivity of relative volatility to pressure, it is shown that controlling the bottom-tray pressure instead of the top-tray pressure leads to operation at the minimum possible average column pressure, so that significant energy savings can be achieved.

General information
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Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CP Kelco ApS
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Redox biocatalysis is currently gaining focus because it offers exquisite selectivity using mild oxidants, such as oxygen (which is environmentally benign). However, it is often challenging to implement oxidative reactions at scale due to the low activity and stability of the biocatalyst under industrial conditions. Consequently, it becomes critical to identify the bottlenecks for specific oxidation reactions as a first step in scale-up. Subsequently, we can identify where research effort is required when developing a biocatalytic reaction for implementation in an industrial reaction, i.e., on biocatalyst development (e.g., improvement of expression levels), process development (e.g., improved oxygen supply, product
removal strategies) or biocatalyst stabilization (e.g. through immobilization or directed evolution). This paper presents a systematic method to identify the bottleneck of a potential biocatalytic process using a monoamine oxidase to synthesise an intermediate in the manufacture of a drug for treating Hepatitis C (Telaprevir).

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.744 SNIP 1.044 CiteScore 2.5
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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
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.797 SNIP 1.032
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.898 SNIP 1.136
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.975 SNIP 1.021
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.835 SNIP 1.007
Scopus rating (2006): SJR 0.723 SNIP 1.069
Scopus rating (2005): SJR 0.742 SNIP 0.955
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.574 SNIP 0.782
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.585 SNIP 0.856
Scopus rating (2002): SJR 0.599 SNIP 0.788
Process intensification in integrated membrane processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technische Universität Dortmund
Authors: Lutze, P. (Ekstern), Gani, R. (Intern)
Pages: 25-57
Publication date: 2014

Host publication information
Title of host publication: Integrated Membrane Operations
Publisher: Walter de Gruyter
Editors: Cassano, A., Drioli, E.
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Chapter: 2
Main Research Area: Technical/natural sciences
Source: dtu
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Process monitoring and modeling of a continuous pharmaceutical from powder to tablet process Line using a mass & energy balance

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Ghent University
Authors: Beer, T. D. (Ekstern), Mortier, S. T. F. (Ekstern), Gernaey, K. (Intern), Nopens, I. (Ekstern)
Publication date: 2014
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 103604664
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Process synthesis, design and analysis using process-group contribution method
This paper describes the development and application of a framework for synthesis, design, and analysis of chemical and biochemical processes. The framework is based on the principle of group contribution used for prediction of physical properties. The fundamental pillars of this methodology are the definition and use of process-groups (building blocks) representing process operations, flowsheet connectivity rules to join the process-groups and flowsheet property models to evaluate the performance of the flowsheet structures. This framework for synthesis and design of chemical and biochemical processes along with the associated models and tools is generic and can be applied either to retrofit problems where improvement of an existing process flowsheet is desired or to design a new process flowsheet. Based on the framework, a prototype software has been developed and its application is highlighted through a case study involving the well-known HDA process. © 2014 Elsevier B.V.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Kumar Tula, A. (Intern), Eden, M. R. (Intern), Gani, R. (Intern)
Pages: 453-458
Publication date: 2014
Process Synthesis, Design and Analysis using Process-Group Contribution Method

Process synthesis implies the investigation of chemical reactions needed to produce the desired product, selection of the separation techniques needed for downstream processing, as well as making decisions on sequencing the involved reaction and separation operations. This work highlights the development of computer aided methodology for fast, reliable and consistent generation of process flowsheets and rank them based on various flowsheet performance indices. This Computer Aided Flowsheet Design methodology is a hybrid approach[1] that combines the physical insights of the knowledge based methods [2] with mathematical programming techniques [3] to formulate and solve a superstructure based optimization problem.

General information
State: Published
Product Design – From Molecules to Formulations to Devices

Product design is a multidisciplinary and diverse subject. This article focuses on product conceptualization (what-to-make) and briefly reviews the corresponding manufacturing processes (how-to-make). Four product types are considered – molecular products, formulated products, devices and functional products. For molecular products, computer-aided design tools are used to predict the physicochemical properties of single molecules and blends. For formulated products, an integrated experiment-molecular modelling approach to generate the formula with the specified product attributes is followed. For devices and functional products, conceptual product design is carried out by modelling the product based on thermodynamics, kinetics and transport processes, by performing experiments, and by decision making based on experience. The results are product specifications in terms of the type of ingredients, composition, and form, shape or configuration of the product. Also discussed are the special considerations in process design to meet the demand on product qualities for devices and functional products.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Hong Kong University of Science and Technology
Authors: Gani, R. (Intern), Ng, K. M. (Ekstern)
Number of pages: 16
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Publisher: Elsevier Science
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Main Research Area: Technical/natural sciences
Conceptual product design, Molecular design, Formulated product, Chemical device, Functional products
Source: PublicationPreSubmission
Source-ID: 102120292
Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

Programming language and tools for Multipurpose Lab-on-a-Chip Platforms

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science , Embedded Systems Engineering, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Technical University of Denmark
Authors: Pop, P. (Intern), Madsen, J. (Intern), Understrup, K. (Ekstern), Alistar, M. (Intern), Minhass, W. H. (Intern), Krühne, U. (Intern)
Number of pages: 1
Publication date: 2014
Event: Poster session presented at 6th Annual Lab-on-a-Chip European Congress, Berlin, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
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Bibliographical note
Poster presentation at Lab-on-a-Chip European Congress, 2014
Source: dtu
Source-ID: u::10992
Publication: Research - peer-review › Poster – Annual report year: 2014
Reflections on the aerobic fermentation stoichiometry of Crabtree positive yeasts

In this communication a stoichiometric steady state model for Crabtree positive yeasts is proposed. The model is sufficiently simple to be corroborated by experimental data on the key metabolic events around Dcrit. The key feature of the model is that the bottleneck aperture for biomass production in the model of Sonnleitner and Käppeli, 1986 shrinks abruptly at Dcrit and continues to decrease with increasing dilution rate. A black box stoichiometric analysis of experiments reported in literature indicates that production of acetaldehyde might account for the abrupt shrinkage through a severe poisoning effect on the respiratory system.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Computer Aided Process Engineering Center
Authors: Villadsen, J. (Intern), Jørgensen, S. B. (Intern)
Pages: 632-637
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Main Research Area: Technical/natural sciences

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Journal: Biotechnology and Bioengineering (Print)
Volume: 111
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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 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
Representing Operational Knowledge of PWR Plant by Using Multilevel Flow Modelling

The aim of this paper is to explore the capability of representing operational knowledge by using Multilevel Flow Modelling (MFM) methodology. The paper demonstrates how the operational knowledge can be inserted into the MFM models and be used to evaluate the plant state, identify the current situation and support operational decisions. This paper will provide a general MFM model of the primary side in a standard Westinghouse Pressurized Water Reactor (PWR) system including sub-systems of Reactor Coolant System, Rod Control System, Chemical and Volume Control System, and emergency heat removal systems. And the sub-systems’ functions will be decomposed into sub-models according to different operational situations. An operational model will be developed based on the operating procedure by using MFM symbols and this model can be used to implement coordination rules for organizing the utilization of different MFM models in different situations. Combining the operational model and different process models, MFM can be used to identify plant situation.

General information
State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Center for Electric Power and Energy, Energy system operation and management, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Safepark Consultancy
Authors: Zhang, X. (Intern), Lind, M. (Intern), Jørgensen, S. B. (Intern), Jensen, N. (Ekstern), Ravn, O. (Intern)
Number of pages: 9
Publication date: 2014

Host publication information
Title of host publication: Proceedings of ISOFIC/ISSNP 2014
Main Research Area: Technical/natural sciences
Multilevel Flow Modelling, Operation Knowledge Reorientation, PWR primary system
Source: PublicationPreSubmission
Source-ID: 104398341
Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

Selections of minimal conditions for a simple intensification and scale up of w-transaminase reactions
A step wise decision matrix is presented to quickly evaluate w-transaminase for a ‘simple scale up’ in the synthetic direction. Here a ‘simple scale up’ is defined as a system without specialized equipment or process development, thus a rapid implementation. The three step method consists of: 1. thermodynamic evaluation, 2. biocatalyst screen and 3. inhibition characterization. Each step of the method has a cut off value for ease implementation. Demonstrated by a case study which eliminated reaction pair candidates based on the cut off criteria. Finally, the most promising candidate was intensified.
Sensor equipment for quantification of spatial heterogeneity in large bioreactor

Suspension cultivation in large stirred tank reactors suffers from imperfect mixing and pressure gradients due to the large size of the liquid column in the bioreactors. This leads to gradients of substrate concentrations and in turn cell population heterogeneity. The processes in large scale cannot be directly compared to laboratory scale experiments due to these reasons, and thus, in order to understand the large scale processes, experimental data has to be collected at large scale. The cost of acquiring data at large scale is high. The bioreactors are usually run with a limited array of sensors and in order to apply more sensor equipment the bioreactor has to be modified which is both costly and results in production downtime. The presence of three phases (gas, liquid, and solid), and the opaque nature of the fermentation broth together with the necessity of heat sterilization further increases the requirements to the sensor equipment. In order to address these issues this study aims to make an investigation into freely floating, battery driven sensor particles that can follow the liquid movement in the reactor and make measurements while being distributed in the whole volume of the bioreactor. The method leaves a minimal footprint and can be applied to running production to gather large scale fermentation data, without the need of dedicated experimental cultivations. Ultimately, data describing the spatial heterogeneity can be used to enhance existing process models and to create better scale - down strategies for lab - scale experiments. Accurate process models and lab - scale experiments could in turn lead to a more scientific approach to scaling of biotechnological processes.

Shape optimisation of a microreactor for biocatalytic synthesis of optically pure chiral amines

Significance of settling model structures and parameter subsets in modelling WWTPs under wet-weather flow and filamentous bulking conditions.

Current research focuses on predicting and mitigating the impacts of high hydraulic loadings on centralized wastewater treatment plants (WWTPs) under wet-weather conditions. The maximum permissible inflow to WWTPs depends not only
on the settleability of activated sludge in secondary settling tanks (SSTs) but also on the hydraulic behaviour of SSTs. The present study investigates the impacts of ideal and non-ideal flow (dry and wet weather) and settling (good settling and bulking) boundary conditions on the sensitivity of WWTP model outputs to uncertainties intrinsic to the one-dimensional (1-D) SST model structures and parameters. We identify the critical sources of uncertainty in WWTP models through global sensitivity analysis (GSA) using the Benchmark simulation model No. 1 in combination with first- and second-order 1-D SST models. The results obtained illustrate that the contribution of settling parameters to the total variance of the key WWTP process outputs significantly depends on the influent flow and settling conditions. The magnitude of the impact is found to vary, depending on which type of 1-D SST model is used. Therefore, we identify and recommend potential parameter subsets for WWTP model calibration, and propose optimal choice of 1-D SST models under different flow and settling boundary conditions. Additionally, the hydraulic parameters in the second-order SST model are found significant under dynamic wet-weather flow conditions. These results highlight the importance of developing a more mechanistic based flow-dependent hydraulic sub-model in second-order 1-D SST models in the future.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Ramin, E. (Intern), Sin, G. (Intern), Mikkelsen, P. S. (Intern), Plósz, B. G. (Intern)
Number of pages: 13
Pages: 209-221
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Water Research
Volume: 63
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Ratings:
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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
Superstructure Development and Optimization under Uncertainty for Design & Retrofit of Municipal Wastewater Treatment Plants.

In this contribution, an optimization-based approach is presented for optimal process selection and design for domestic wastewater treatment plants (WWTPs). In particular, we address the issue of uncertainties by formulating the WWTP design problem as a Stochastic Mixed Integer (Non) Linear Programming (sMI (N) LP) problem, which is then solved to determine the optimal process selection and flow diagram (i.e., the interconnection between process units) that meet a set of performance criteria including effluent quality requirements, cost, and technical requirements. The application of the framework is highlighted using a case study aiming at designing a new WWTP under different objective function scenarios. For the uncertainty analysis, sources related to influent wastewater composition, operational cost, and effluent permit requirements are studied, and robust design candidates are generated and discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Bozkurt, H. (Intern), Quaglia, A. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Pages: 37–42
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Computer - Aided Chemical Engineering
Volume: 33
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Ratings:
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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
In this contribution, an optimization-based approach is presented for optimal process selection and design for domestic wastewater treatment plants (WWTPs). In particular, we address the issue of uncertainties by formulating the WWTP design problem as a Stochastic Mixed Integer (Non) Linear Programming (sMI (N) LP) problem and solve it to determine the optimal process selection and flow diagram that meet a set of performance criteria including effluent quality requirements, cost and technical requirements. The application of the framework is highlighted using a case study aiming at designing a new WWTP under different objective function scenarios. For the uncertainty analysis, sources related to influent wastewater composition, operational cost and effluent permit requirements are studied and robust design candidates are generated and discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Bozkurt, H. (Intern), Quaglia, A. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Number of pages: 6
Publication date: 2014

Host publication information
Title of host publication: Proceedings of the 24th European Symposium on Computer Aided Process Engineering
Publisher: Elsevier Science
Main Research Area: Technical/natural sciences
Design, Modelling, Superstructure optimization, Uncertainty analysis, Wastewater treatment
Source: PublicationPreSubmission
Source-ID: 103645718
Publication: Research - peer-review › Article in proceedings – Annual report year: 2014
Sustainable Process Networks for CO2 Conversion

According to various organizations, especially the Intergovernmental Panel on Climate Change, global warming is an ever-increasing threat to the environment and poses a problem if not addressed. As a result, efforts are being made across academic and industrial fields to find methods of reducing contributors to global warming, primarily greenhouse gas emissions. Of these, carbon dioxide (CO2) is the largest source and, therefore, the reduction of the amount emitted is primary focus of developments [1]. Currently, the main method that is focused on is carbon capture and storage (CCS). There are various drawbacks to this geologic storage system: the CO2 is not eliminated, the implementation is limited due to natural phenomena, and the capturing methods are often expensive. Thus, it is desirable to develop an alternative strategy for reducing the CO2 emissions [2]. An additional process that reduces the emissions is the conversion of CO2 into useful products, such as methanol [3]. In this work, through a computer-aided framework for process network synthesis-design, a network of feasible conversion processes that all use emitted CO2 is investigated. CO2 is emitted into the environment from various sources: power generation, industrial processes, transportation and commercial processes. Within these there are high-purity emissions and low-purity emissions. Rather than sending these to the atmosphere, it is possible to collect them and use them for other purposes. In this work, the first step is determining the various CO2-sources, the amounts emitted, and the corresponding compositions. These sources show large variations in amounts and concentrations. Targeting some of the largest contributors: power generation, manufacturing, chemical industry, it is possible to determine the amounts available. Transportation and other sources are more difficult to capture and utilize further and, therefore, they are not considered in this work. Once the CO2-sources are known, it is possible to determine how to utilize these through process network optimization. It is then necessary to have the information on the conversions that are thermodynamically feasible, including the co-reactants, catalysts, operating conditions and reactions. Research has revealed that there are a variety of reactions that fulfill the aforementioned criteria. The products that are formed fall into categories: fuels, bulk chemicals and specialty chemicals. While fuels, such as methanol (MeOH) have the largest market, this network will include a variety of thermodynamically feasible conversion paths [4]. From reviews of work previously done, there are ranges of possible products that are formed from CO2 and another co-reactant directly. Methanol, dimethyl ether, dimethyl carbonate and ethylene carbonate are just some of the possible products that can be formed. Each of these involves CO2 and a co-reactant, such as hydrogen, which may also be captured from process purge streams. The process network evolves as some of the reactions involve products from other reactions as a reactant. Combining the possible products that can be formed and the reactants that are required yields a network of products that can be created using only the CO2 emissions and not adding any CO2 emissions through the reactions. Using the computer-aided framework, the feasible networks are generated and simulated to verify the initial synthesis design results. The economic feasibility and sustainability are assessed to identify the final, more sustainable network. The goal is to create a network that reduces emissions by forming desirable chemical products without emitting noticeable amounts of CO2 and other greenhouse gases, and creating more energy efficient processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Chulalongkorn University
Authors: Frauzem, R. (Intern), Kongpanna, P. (Ekstern), Pavarajam, V. (Ekstern), Gani, R. (Intern), Assabumrungrat, S. (Ekstern)
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences
Electronic versions: AIChE_Abstract.docx
Source: PublicationPreSubmission
Source-ID: 103645414
Publication: Research - peer-review » Conference abstract for conference – Annual report year: 2014

Sustainable Process Synthesis-Intensification

Sustainable process design can be achieved by performing process synthesis and process intensification together. This approach first defines a design target through a sustainability analysis and then finds design alternatives that match the target through process intensification. A systematic, multi-stage framework for process synthesis-intensification that identifies more sustainable process designs has been developed. At stages 1-2, the working scale is at the level of unit operations, where a base case design is identified and analyzed with respect to sustainability metrics. At stages 3-4, the working scales are at the levels of unit operations, tasks and phenomena. Here, first intensified flowsheet alternatives are generated through a task-based process synthesis method where tasks performed in unit operations are identified, analyzed and recombined through a means-ends analysis. Next, a phenomena-based process synthesis method is applied, where the phenomena involved in each tasks are identified, manipulated and recombined to generate new and/or existing unit operations configured into flowsheets that are more sustainable from those found in the previous levels. An overview of the key concepts and the 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 dimethyl carbonate.

General information
State: Published
The chemical and biochemical industry needs major reductions in energy consumption, waste generation, number of equipment used in the construction of plants and capital/operational cost. These required reductions can be addressed through process intensification that is the efficient use of raw materials (feedstock) and the use of sustainable technologies or processes which directly impacts and improves sustainability/LCA factors. Process intensification is a concept by which processes, whether conceptual or existing, can be designed or redesigned to achieve more efficient and sustainable designs. Therefore sustainable process design can be achieved by performing process synthesis and process

Sustainable Process Synthesis-Intensification
The chemical and biochemical industry needs major reductions in energy consumption, waste generation, number of equipment used in the construction of plants and capital/operational cost. These required reductions can be addressed through process intensification that is the efficient use of raw materials (feedstock) and the use of sustainable technologies or processes which directly impacts and improves sustainability/LCA factors. Process intensification is a concept by which processes, whether conceptual or existing, can be designed or redesigned to achieve more efficient and sustainable designs. Therefore sustainable process design can be achieved by performing process synthesis and process
The main contribution of this work is the development of a systematic computer-aided multi-scale, multi-level framework for performing process synthesis-intensification that aims to make a process more sustainable than a base case design, which represents either a new or existing process. The framework consists of eight steps (step 1 to step 8) that operates at the unit operation scale and task scale, and four integrated task-phenomena-based steps (IT-PBS.1 to IT-PBS.4) that operates at the task scale and phenomena scale. The concept of generating more sustainable designs through the combination of phenomena provides the opportunity to innovate through the generation of novel unit operations and thereby expand the search space of available unit operations. At the unit operations scale a conceptual base case design is synthesized through the sequencing of unit operations. The base case is then designed and analysed for identifying process limitations or bottlenecks (hot-spots) using a comprehensive analysis consisting of economic, life cycle and sustainability analyses that are translated into design targets. These hot-spots are associated with tasks that may be targeted for overall process improvement. Next an integrated task-phenomena-based synthesis method is applied, where the involved phenomena in various tasks are identified, manipulated and recombined using combination rules in order to generate new and/or existing unit operations that are configured into flowsheet alternatives inclusive of hybrid/intensified unit operations. The flowsheet alternatives that satisfy the performance criteria and design targets, give innovative and more sustainable, non-trade off flowsheet designs that otherwise could not be found from the higher scales. The framework is applied to three case studies related to the chemical and bioprocess industry in order to test the applicability of the framework for covering a wide range of applications, showing that process intensification provides major benefits related to the generation of more sustainable process designs.
Systematic Chemical Process Design: Sustainable Production of Formaldehyde from Natural Gas

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Lydom, S. I. (Ekstern), Mortensen, S. (Ekstern), Pedersen, P. N. (Ekstern), Papadakis, E. (Intern)
Number of pages: 1
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences
Electronic versions: Systematic_Chemical_Process_Design.pdf

Systematic computer aided framework for process synthesis, design and intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern), Babi, D. K. (Intern)
Pages: 698-751
Publication date: 2014

Host publication information
Title of host publication: Chemical Processes for a Sustainable Future
Publisher: Royal Society of Chemistry
Editors: Letcher, T., Scott, J., Patterson, D. A.
ISBN (Print): 978-1-84973-975-7
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 104283711
Publication: Research - peer-review › Book chapter – Annual report year: 2014

The focus of this work is on process systems engineering (PSE) methods and tools, and especially on how such PSE methods and tools can be used to accelerate and support systematic bioprocess development at a miniature scale. After a short presentation of the PSE methods and the bioprocess development drivers, three case studies are presented. In the first example it is demonstrated how experimental investigations of the bi-enzymatic production of lactobionic acid can be modeled with help of a new mechanistic mathematical model. The reaction was performed at lab scale and the prediction quality analyzed. In the second example a computational fluid dynamic (CFD) model is used to study mass transfer phenomena in a microreactor. In this example the model is not only used to predict the transient dynamics of the reactor system but also to extract material properties like the diffusion velocities of substrate and product, which is otherwise difficult to access. In the last example, a new approach to the design of microbioreactor layouts using topology optimization is presented and discussed. Finally, the PSE methods are carefully discussed with respect to the complexity of the presented approaches, the applicability with respect to practical considerations and the opportunity to analyze experimental results and transfer the knowledge between different scales.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Process Engineering and Technology
Authors: Krühne, U. (Intern), Larsson, H. (Intern), Heintz, S. (Intern), Ringborg, R. H. (Intern), Pereira Rosinha, I. (Intern), Bodla, V. K. (Intern), Andrade Santacoloma, P. D. G. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern), Gernaey, K. (Intern)
Pages: 203-214
Systematic Methodology for Design of Tailor-Made Blended Products: Fuels and Other Blended Products

A tailor-made blended liquid product is defined as a formulation of various chemicals in the liquid state to obtain a liquid mixture with a specific set of desired characteristics and qualities. Examples of blended liquid products are synthetic fuels and lubricants. This type of products is very important in daily life, since they not only keep people moving around, but also guarantee that machines and equipment work smoothly. The objective of this work is to tackle the blending problems...
using computer-aided tools for the initial stage of the product design. A systematic methodology for design of tailor-made blended products has been developed, which has four main tasks. First, the design problem is defined: the product needs are identified, translated into target properties and the bounds for each target property are defined. Secondly, target property models are retrieved from a property model library. Thirdly, a mixture/blend design algorithm is applied to obtain the mixtures/blends that match the design targets. The result is a set of blends that match the constraints, the composition of the chemicals present in the blend, and the values of the target properties. Finally, the mixture target property values are verified by means of rigorous models for the properties and the mixtures. Besides the methodology, as the main contribution, specific supporting tools that were developed to perform each task are also important contributions of this research work. The applicability of the developed methodology and tools was tested through two case studies. In the first case study, two different gasoline blend problems have been solved. In the second case study, four different lubricant design problems have been solved.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. B. (Intern), Gani, R. (Intern), Gernaey, K. (Intern), Woodley, J. M. (Ekstern)
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Publication date: 2014

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Publisher: Technical University of Denmark, Department of Chemical and Biochemical Engineering
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Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Systematic_Methodology_for_Design.pdf
Publication: Research › Ph.D. thesis – Annual report year: 2014

**Systematic Process Design and Operation of Intensified Processes**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Mansouri, S. S. (Intern), Huusom, J. K. (Intern), Woodley, J. M. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
362191_Systematic_Process_Design.pdf
Source: PublicationPreSubmission
Source-ID: 102790390
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

**Techno-economic assessment of FT unit for synthetic diesel production in existing stand-alone biomass gasification plant using process simulation tool**

For alternative thermo-chemical conversion process route via gasification, biomass can be gasified to produce syngas (mainly CO and H2). On more applications of utilization, syngas can be used to synthesize fuels through the catalytic process option for producing synthetic liquid fuels such as Fischer-Tropsch (FT) diesel. The embedding of the FT plant into the stand-alone based on power mode plants for production of a synthetic fuel is a promising practice, which requires an extensive adaptation of conventional techniques to the special chemical needs found in a gasified biomass. Because there are currently no plans to engage the FT process in Thailand, the authors have targeted that this work focus on improving the FT configurations in existing biomass gasification facilities (10 MWh). A process simulation model for calculating extended unit operations in a demonstrative context is designed by commercial software. The aim of this work is to develop detailed process flow diagram for the FT technology in order to subsequently study the economic feasibility based on once-Through mode. A cost analysis is performed to find out the convenience of the proposed solutions.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, King Mongkut's University of Technology Thonburi, National Metal and Materials Technology Center
Authors: Hunpinyo, P. (Ekstern), Narataruksa, P. (Ekstern), Tungkamani, S. (Ekstern), Chollacoop, N. (Ekstern), Cheali, P. (Intern)
Nowadays, companies are looking for new sustainable design alternatives that improve their original processes. To assess the best design alternative, economic aspects have been the preferred indicators. However, environmental and social concerns should also be included in the decision process so that truly sustainable design alternatives can be found. This work proposes a framework, called ‘Techno-Economic Sustainability Environmental Impact Diagnosis’ (TESED) that allows users to assess chemical/biochemical processes in a product oriented analysis. TESED is a systematic and generic approach that can be applied to any product/processes combination. Bioethanol production was the case-study selected to highlight the TESED framework. Two production processes using two different feedstocks, hardwood chips and cassava rhizome, have been analysed.
The Electrical Breakdown of Thin Dielectric Elastomers: Thermal Effects

Dielectric elastomers are being developed for use in actuators, sensors and generators to be used in various applications, such as artificial eye lids, pressure sensors and human motion energy generators. In order to obtain maximum efficiency, the devices are operated at high electrical fields. This increases the likelihood for electrical breakdown significantly. Hence, for many applications the performance of the dielectric elastomers is limited by this risk of failure, which is triggered by several factors. Amongst others thermal effects may strongly influence the electrical breakdown strength. In this study, we model the electrothermal breakdown in thin PDMS based dielectric elastomers in order to evaluate the thermal mechanisms behind the electrical failures. The objective is to predict the operation range of PDMS based dielectric elastomers with respect to the temperature at given electric field. We performed numerical analysis with a quasi-steady state approximation to predict thermal runaway of dielectric elastomer films. We also studied experimentally the effect of temperature on dielectric properties of different PDMS dielectric elastomers. Different films with different percentages of silica and permittivity enhancing filler were selected for the measurements. From the modeling based on the fitting of experimental data, it is found that the electrothermal breakdown of the materials is strongly influenced by the increase in both dielectric permittivity and conductivity.
The need and challenge to find more sustainable alternatives for the modern society

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern)
Publication date: 2014
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 103564428
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

The Optimization-Based Design and Synthesis of Water Network for Water Management in an Industrial Process: Refinery Effluent Treatment Plant

The increasing awareness of the sustainability of water resources has become an important issue. Many process industries contribute to high water consumption and wastewater generation. Problems in industrial water management include the processing of complex contaminants in wastewater, selection of wastewater treatment technologies, as well as water allocation, limited reuse, and recycling strategies. Therefore, a water and wastewater treatment network design requires the integration of both economic and environmental perspectives. The aim of this work was to modify and develop a generic model-based synthesis process for a water/wastewater treatment network design problem utilizing the framework of Quaglia et al. (2013) in order to effectively design, synthesize, and optimize an industrial water management problem using different scenarios (both existing and retrofit system design). The model-based mathematical problem was formulated as mixed integer linear (MILP) and mixed integer non-linear programming (MINLP) and strived to identify the best wastewater treatment processes among a set of predefined alternatives that produce a minimum total annualized cost, while meeting all wastewater specification criteria. In addition, the effluent options (for different retrofit scenarios) in the modified superstructure could be set as discharge only, zero liquid discharge (total recycling), or a combination of recycling and discharge with the aim of minimizing the amount of fresh process water consumption through the recycling of treated wastewater. Also, an industrial case study of a refinery wastewater treatment plant was implemented. Alternative recycling schemes (retrofit design problem) were proposed and solved. The retrofit design solution using developed generic model-based synthesis offered a preliminary guideline for a better wastewater treatment network in terms of economic benefits and environmental impact compared to the existing process and accomplished it in an effective time frame.

General information
Thermodynamic Evaluation of the Production of Chiral Amines from Long-Chain Aliphatic Alcohols

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Abu, R. (Intern), Lima Ramos, J. (Intern), Woodley, J. (Intern)
Publication date: 2014
Main Research Area: Technical/natural sciences
Electronic versions:
MECP14_Abu_et_al._2014_.pdf
Source: PublicationPreSubmission
Source-ID: 103263552
Publication: Research - peer-review › Poster – Annual report year: 2014

The Virtual Product-Process Design Lab

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Authors: Kalakul, S. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
AICHE_sawit_abstract.pdf
Source: PublicationPreSubmission
Source-ID: 103645344
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

The Virtual Product-Process Design Laboratory for Structured Chemical Product Design and Analysis
The objective of this paper is to present new methods for design of chemicals based formulated products and their implementation in the software, the Virtual Product-Process Design Laboratory. The new products are tailor-made blended liquid products and emulsion-based products. The new software employs a template approach, where each template follows the same common steps in the workflow for design of formulated products, but has the option to employ different product specific property models, data and calculation routines, when necessary. With the new additions, the software is able to support the design and analysis of a wide range of homogeneous formulated products: tailor-made blends, single phase liquid formulations and emulsion-based products. The decision making process is supported by dedicated property models and structured databases, specifically developed for each design problem scenario. Output from the software is a small set of most promising product candidates and a short list of recommended experiments that can validate and further
fine-tune the product composition. The application of the new features is highlighted through two case studies relative to an emulsion-based product and a tailor-made blend.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Authors: Mattei, M. (Intern), Yunus, N. A. B. (Intern), Kalakul, S. (Intern), Kontogeorgis, G. (Intern), Woodley, J. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Pages: 61-66
Publication date: 2014

**Host publication information**
Publisher: Elsevier Science
Main Research Area: Technical/natural sciences
Product Design, Formulation Design, Blend Design, Emulsion Design
DOIs: 10.1016/b978-0-444-63456-6.50011-9
Source: PublicationPreSubmission
Source-ID: 102119457
Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

**Tools to prevent process safety events at university research facility - chemical risk assessment and experimental set-up risk assessment.**
The article discusses the two forms developed to examine the hazards of the chemicals to be used in the experiments in the experimental setup in the Department of Chemical and Biochemical Engineering of the Technical University of Denmark. A system for the safety assessment of new experimental setups in university research and teaching laboratories is presented. The significance of the forms for the effort of researchers in improving work with significant hazards is described.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Safepark Consultancy
Authors: Jensen, N. (Intern), Jørgensen, S. B. (Intern)
Pages: 25-28
Publication date: 2014
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Loss Prevention Bulletin
Issue number: 238
ISSN (Print): 0260-9576
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Original language: English
DANMARKS tekniske universitet
Source: FindIt
Source-ID: 270431217
Publication: Research - peer-review › Journal article – Annual report year: 2014

**Toward a Computer-Aided Synthesis and Design of Biorefinery Networks: Data Collection and Management Using a Generic Modeling Approach**
Recent research into biorefineries resulted in many competing concepts and technologies for conversion of renewable biobased feedstock into an array of promising products including fuels, chemicals, materials, etc. The topic of this study is collection and management of the complex biorefinery data that are needed among others to support the superstructure-based optimization studies. To this end, we first formulate an integrated thermochemical and biochemical biorefinery superstructure and then use a generic modeling approach to represent each processing technology in the superstructure. The generic model parameters includes reaction yield, utility consumption, and separation efficiency among others, which are identified on the basis of input-output data (generated from rigorous models) collected from detailed biorefinery case studies reported in the open literature. The outcome is a verified database for the extended biorefinery networks.
combining thermochemical and biochemical platforms that represents 2882 potential biorefinery routes. The validated biorefinery database is made public and can be used to cross-validate and benchmark new biorefinery technologies and concepts as well as in superstructure-based optimization studies.

Towards a single empirical correlation to predict kLa across scales and processes

Mathematical models are increasingly used in fermentation. Nevertheless, one of the major limitations of these models is that the parameters they include are process specific, e.g. the volumetric mass transfer coefficient (kLa). Oxygen transfer was studied in order to establish a single equation to predict kLa, and data from a range of processes – pilot and production scale – were extracted. On-line viscosity was measured for all processes (56 batches). Off-line rheological measurements were performed for the pilot scale processes (26 batches). The apparent viscosity was evaluated with 5 different calculations of the average shear rate. The experimental kLa value was determined with the direct method; however, eight variations of its calculation were evaluated. Several simple correlations were fitted to the measured kLa data. The standard empirical equation was found to be best for predicting kLa in all processes at pilot scale using off-line viscosity measurements, and using the equation from Henzler and Kauling (1985) to evaluate the shear rate. In addition, a parameter set of the standard empirical equation was found that can predict oxygen transfer in Bacillus processes at all scales using on-line viscosity measurements. A single correlation for all processes and all scales could not be established.
Towards BSM2-GPS-X: A plant-wide benchmark simulation model not only for carbon and nitrogen, but also for greenhouse gases (G), phosphorus (P), sulphur (S) and micropolllutants (X), all within the fence of WWTPs/WRRFs

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Lund University, University of Navarra, University of Cape Town, Universite Laval, University of Queensland, University of KwaZulu-Natal, Dynamita
Pages: 123-128
Publication date: 2014

Host publication information
Title of host publication: Proceedings. 4th IWA/WEF Wastewater treatment modelling seminar
Publisher: Water Environment Federation
Main Research Area: Technical/natural sciences
Conference: 4th IWA/WEF Wastewater Treatment Modelling Seminar 2014, Spa, Belgium, 30/03/2014 - 30/03/2014
Electronic versions: PRO14_37.pdf

Toxicity of nonylphenol diethoxylate in lab-scale anaerobic digesters
Nonylphenol compounds have high commercial, industrial and domestic uses owing to their surface active properties. In addition to their toxic, carcinogenic and persistent characteristics; they have drawn the attention of scientists lately due to their endocrine disrupting properties. Their widespread use and disposal cause them to enter wastewater treatment systems at high concentrations. Since they are highly persistent and hydrophobic, they accumulate mostly on sludge. In this study using Anaerobic Toxicity Assay (ATA) tests, the toxicity of a model nonylphenol compound, nonylphenol diethoxylate (NP2EO), for anaerobic digestion of sludge was determined. The test bottles were dosed with NP2EO in acetone, with concentrations ranging from 1mgL-1 to 30mgL-1. During the tests, gas productions and compositions in terms of methane and carbon dioxide were monitored. To be able to judge about the fate, the target compounds were extracted from water and sludge and analyzed using GC/MS. The sludge samples used for assembling the reactors were found to contain NP and NP1EO but no NP2EO. After the assay was completed, all the NP2EO spiked into the live reactors was found to disappear. The increase seen in NP1EO and NP and further accumulation of NP in the system, indicated the conversion of NP2EO to these metabolites. On the other hand, no conversion was observed in abiotic reactors. Inhibition of NP2EO for anaerobic microorganisms was not observed throughout the tests considering the biogas production of the test reactors in comparison to the control reactors. © 2013 Elsevier Ltd.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Middle East Technical University
Authors: Bozkurt, H. (Intern), Sanin, F. D. (Ekstern)
Pages: 69-75
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemosphere
Volume: 104
ISSN (Print): 0045-6535
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Environmental Chemistry, Chemistry (all), Anaerobic digestion, Anaerobic Toxicity Assay test, Nonylphenol compounds,
NP2EO, Sludge, Acetone, Carbon dioxide, Chromatographic analysis, Methane, Phenols, Testing, Wastewater treatment,
Anaerobic microorganisms, Anaerobic toxicity assay tests, Endocrine disrupting properties, Nonylphenols, Surface-active
property, Wastewater treatment system, Toxicity, acetone, carbon dioxide, methane, nonylphenol, nonylphenol
diethoxylate, unclassified drug, anoxic conditions, assay, biogas, bioreactor, concentration (composition), endocrine
disruptor, gas production, metabolite, microbial community, phenolic compound, sludge, toxicity test, waste treatment,
wastewater, anaerobic bacterium, anaerobic digestion, anaerobic reactor, anaerobic toxicity assay test, article, chemical
composition, concentration (parameters), gas, mass fragmentography, sludge treatment, temperature, toxicity testing
Uncertainty analysis in raw material and utility cost of biorefinery synthesis and design
This study presents the impact of uncertain data on the solution obtained by using a superstructure-based optimization approach in synthesis and design of biorefinery processing networks. In the early stages of biorefinery design, many of the data required for the formulation of the design problem are characterized by considerable uncertainty. These uncertainties might have significant impact on the results of the design problem, and therefore need to be carefully evaluated and managed, in order to generate candidates for robust design. In this contribution, we study the effect of data uncertainty (raw material price and utility cost) on the design of a biorefinery process network.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Cheali, P. (Intern), Quaglia, A. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Pages: 49–54
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication Information
Journal: Computer - Aided Chemical Engineering
Volume: 33
ISSN (Print): 1570-7946
Ratings:
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
Scopus rating (2007): SJR 0.182 SNIP 0.094
Scopus rating (2006): SJR 0.138 SNIP 0.108
Scopus rating (2005): SJR 0.178 SNIP 0.178
Scopus rating (2004): SJR 0.19 SNIP 0.161
Scopus rating (2003): SJR 0.157 SNIP 0.212
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.168 SNIP 0.214
Scopus rating (2001): SJR 0.146 SNIP 0.193
Scopus rating (2000): SJR 0.102 SNIP 0
Scopus rating (1999): SJR 0.102 SNIP 0
μ-structured devices as tools for screening process intensification in biocatalysis

Biocatalytic processes have been emerging as potential replacements of traditional chemical synthesis in many industrial relevant production processes. However the implementation of new biocatalytic processes can be a very challenging procedure which requires both biocatalyst and process screening and characterization for economic evaluation before scale-up. Microstructured devices have been used as screening tools that allow paradigm changes in process development by shortening process development times through modularity and intensification. Customized reactor designs and process configurations by integrating different modules can be developed at microscale. Such configurations enable effective screening and rapid process development of biocatalytic reactions assuring economic viability and shorter time to market for pharmaceutical products. Thus the work presented in this thesis is based on the application of microstructured devices for screening and characterization of process options in biocatalytic processes. The thesis focuses on interesting case studies like the asymmetric synthesis of chiral amines using ω-transaminases and synthesis of an industrially relevant imine product using monoamine oxidase. The first part of the thesis is focused on the development of novel reactor configurations for biocatalysis. A combination of micro reactors and computational fluid dynamics (CFD) has been found to contribute significantly towards the understanding of diffusional properties of the substrate and the product. Such knowledge is subsequently applied to design customized reactor configurations. It has been demonstrated that this knowledge can be crucial for the choice and design of reactors. The second part focuses on developing μ-scale modules for rapid screening and integrating process units. The increase in productivity is evaluated through process metrics. A case study demonstrates the applicability of using a micro-scale packed bed column for screening synthetic resins for in-situ product removal. CFD simulations were performed to guide the design of a packed column for efficient operation. Further case studies demonstrate the development of modular set-ups with integrated processes at microscale to address process limitations which were determined by initial experiments at lab scale. The degree of integration of functionalities requires process optimization. Thus optimization studies were also performed by varying operational parameters. From an academic point of view, a general methodology is desired and thus a systematic screening methodology is proposed that relies on microstructured devices during process development. The methodology can be applied to other biocatalytic
16 Years of Experience with Rule Based Control of Copenhagen's Sewer System
The sewer system in Copenhagen started implementing Real Time Control (RTC) in the 1990's in a small subcatchment. The method used was and still is rule based control. Since then the use of RTC has been expanded to the whole catchment and continuously improved from operational experience. These experiences are shared and put into a framework to be used for a common understanding of the problems that can be solved using rule based control and control in general.
Benefits and limitations of using rule based control are examined and future perspectives of the control structure of Copenhagen are outlined.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering, Urban Water Systems, Lynettefællesskabet I/S, HOFOR A/S
Authors: Mollerup, A. L. (Intern), Thornberg, D. (Ekstern), Mikkelsen, P. S. (Intern), Johansen, N. B. (Ekstern), Sin, G. (Intern)
Number of pages: 4
Publication date: 2013
Event: Abstract from 11th IWA conference on instrumentation control and automation, Narbonne, France.
Main Research Area: Technical/natural sciences
Electronic versions:
2013_Mollerup_et_al._ICA_Narbonne_ExtendedAbstract.pdf
Source: PublicationPreSubmission
Source-ID: 133795269
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

3D modelling of coupled mass and heat transfer of a convection-oven roasting process
A 3D mathematical model of coupled heat and mass transfer describing oven roasting of meat has been developed from first principles. The proposed mechanism for the mass transfer of water is modified and based on a critical literature review of the effect of heat on meat. The model equations are based on a conservation of mass and energy, coupled through Darcy's equations of porous media - the water flow is mainly pressure-driven. The developed model together with theoretical and experimental assessments were used to explain the heat and water transport and the effect of the change in microstructure (permeability, water binding capacity and elastic modulus) that occur during the meat roasting process. The developed coupled partial differential equations were solved by using COMSOL Multiphysics®3.5 and state variables are predicted as functions of both position and time. The proposed mechanism was partially validated by experiments in a convection oven where temperatures were measured online. © 2012 Elsevier Ltd.

General information
State: Published
Organisations: National Food Institute, Division of Industrial Food Research, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Feyissa, A. H. (Intern), Adler-Nissen, J. (Intern), Gernaey, K. (Intern)
Pages: 810-820
Publication date: 2013
Main Research Area: Technical/natural sciences
3D-printer vejen til innovation?

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Technical University of Denmark
Authors: Poulsen, A. (Ekstern), Heintz, S. (Intern), Ringborg, R. H. (Intern), Woodley, J. (Intern), Gernaey, K. (Intern), Krühne, U. (Intern)
Pages: 32-34
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 94
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: Danish
Electronic versions:
Dansk Kemi 3D print.pdf
Source: dtu
Source-ID: u::8887
Publication: Communication › Journal article – Annual report year: 2013

Accelerating Scale-up of Bioprocesses using a Model-based and Multi-objective Optimisation Methodology

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Mauricio Iglesias, M. (Intern), Sin, G. (Intern)
Publication date: 2013
Event: Poster session presented at 9th World Congress of Chemical Engineering Incorporating 15th Asian Pacific Confederation of Chemical Engineering Congress, Seoul, Korea, Republic of.
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9039
Publication: Research - peer-review › Poster – Annual report year: 2013

Achieving More Sustainable Solutions through Process Intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Gani, R. (Intern), Babi, D. K. (Intern), Mansouri, S. S. (Intern), Ismail, M. I. (Ekstern), Huusom, J. K. (Intern), Woodley, J. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from 50th Anniversary Symposium of the Department of Chemical & Biological Engineering, Korea University, Seoul, Korea, Republic of.
A control scheme for filament stretching rheometers with application to polymer melts

We propose a new control scheme to maintain a constant strain rate of the mid-filament diameter in a filament stretching rheometer for polymer melts. The scheme is cast as a velocity algorithm and consists of a feed-back and a feed-forward contribution. The performance of the controller is demonstrated on a commercial low density polyethylene. Several strain rates and experimental conditions are tested to demonstrate the necessity of the control parameters and the limits of both the control scheme and the experimental apparatus. When the control parameters are properly tuned, the algorithm ensures that the applied strain stays within 2% of the set point and measurements can be made up to Hencky strains of 6.5.
Advances in the Process Development of Biocatalytic Processes

Biocatalysis is already established in chemical synthesis on an industrial scale, in particular in the pharmaceutical sector. However, the wider implementation of biocatalysis is currently hindered by the extensive effort required to develop a competitive process. In order that resources spent on development are used in the most efficient manner for these challenging systems, a holistic view on process development and a more in-depth understanding of the underlying constraints (process related as well as biocatalyst related) are required. In this concept article a systematic approach to solve this problem is proposed, involving the use of process tools and methods to assist in development.
A flexible modular process design for enzymatic biodiesel production

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Seita, C. S. (Intern), Nordblad, M. (Intern), Woodley, J. (Intern)
Publication date: 2013
Event: Abstract from 104th AOCS Annual Meeting & Expo, Montreal, Canada.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

A Framework for Process Synthesis integrated with Sustainability and Process Intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Technical University of Dortmund
Authors: Babi, D. K. (Intern), Holtbruegge, J. (Ekstern), Lutze, P. (Ekstern), Woodley, J. (Intern), Górak, A. (Ekstern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2013
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation
Source: dtu
Source-ID: u::9427
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

A future perspective on the role of industrial biotechnology for chemicals production

The development of recombinant DNA technology, the need for renewable raw materials and a green, sustainable profile for future chemical processes have been major drivers in the implementation of industrial biotechnology. The use of
industrial biotechnology for the production of chemicals is well established in the pharmaceutical industry but is moving
down the value chain toward bulk chemicals. Chemical engineers will have an essential role in the development of new
processes where the need is for new design methods for effective implementation, just as much as new technology. Most
interesting is that the design of these processes relies on an integrated approach of biocatalyst and process engineering.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology,
Computer Aided Process Engineering Center, BASF, DSM Chemtech Center
Authors: Woodley, J. (Intern), Breuer, M. (Ekstern), Mink, D. (Ekstern), Gani, R. (ed.) (Intern)
Pages: 2029-2036
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Research and Design
Volume: 91
Issue number: 10
ISSN (Print): 0263-8762
Ratings:
BFI (2018): BFI-level 2
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
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
Web of Science (2005): Indexed yes
A fuzzy-logic based diagnosis and control of a reactor performing complete autotrophic nitrogen removal

Diagnosis and control modules based on fuzzy set theory were tested for novel bioreactor monitoring and control. Two independent modules were used jointly to carry out first the diagnosis of the state of the system and then use transfer this information to control the reactor. The separation in diagnosis and control allowed a more intuitive design of the membership functions and the production rules. Hence, the resulting diagnosis-control module is simple to tune, update and maintain while providing a good control performance. In particular the diagnosis-control system was designed for a complete autotrophic nitrogen removal process. The whole module is evaluated by dynamic simulation.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Mauricio Iglesias, M. (Intern), Vangsgaard, A. K. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Number of pages: 1
Publication date: 2013
Event: Poster session presented at CAB 2013, Mumbai, India.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review • Journal article – Annual report year: 2013

A fuzzy-logic based diagnosis and control of a reactor performing complete autotrophic nitrogen removal

This contribution explores the use of diagnosis and control modules based on fuzzy set theory and logic for bioreactor monitoring and control. With this aim, two independent modules were used jointly to carry out first the diagnosis of the state of the system and then use transfer this information to control the reactor. The separation in diagnosis and control allowed a more intuitive design of the membership functions and the production rules. Hence, the resulting diagnosis-control module is simple to tune, update and maintain while providing a good control performance. In particular the diagnosis-control system was designed for a complete autotrophic nitrogen removal process. The whole module is evaluated by dynamic simulation. Additionally, the diagnosis tool was demonstrated by analysis 100 days of experimental data.

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A Generic Life Cycle Assessment Tool for Chemical-biochemical Processes

As environmental impacts and resource depletion are serious concerns for the modern society, they also provide the motivation and need to design processes that are not only economically and operationally feasible, but also environmentally friendly. In this respect, life cycle assessment (LCA) is a tool for quantifying potential environmental impacts throughout the life cycle of the product or process. It can be used in conjunction with an economic tool to evaluate the design of any existing and/or new chemical-biochemical process and create improvement options in order to arrive at the best design among various alternatives. Although there are several commercial LCA software, there is still need to for a simple LCA software that can be integrated with process design tools. The objective of this paper is to present a new LCA software, LCSoft, which is exclusively designed for chemical-biochemical processes and integrated with other design tools. LCSoft has the following highlights: (1) database of collected environmental properties and other parameters needed for calculation of LCA indices and environmental impacts; (2) a group contribution+ method (GC+) for the accurate estimation of environmental factors; (3) integration with an economic analysis software, ECON; (4) integration with sustainable process design software, SustainPro; and, (5) efficient and systematic work-flow for the calculation of impacts and assessment parameters. LCSoft has been tested on several chemical and biochemical processes. In this paper, the application of LCSoft to the analysis of the NREL bioethanol process will be presented and compared with other LCA based software.

A GLUE uncertainty analysis of a drying model of pharmaceutical granules

A shift from batch processing towards continuous processing is of interest in the pharmaceutical industry. However, this transition requires detailed knowledge and process understanding of all consecutive unit operations in a continuous manufacturing line to design adequate control strategies. This can be facilitated by developing mechanistic models of the multi-phase systems in the process. Since modelling efforts only started recently in this field, uncertainties about the model predictions are generally neglected. However, model predictions have an inherent uncertainty (i.e. prediction uncertainty) originating from uncertainty in input data, model parameters, model structure, boundary conditions and software. In this paper, the model prediction uncertainty is evaluated for a model describing the drying behaviour of a single pharmaceutical granule in two consecutive phases is used. First of all, the effect of the assumptions at the particle level on the prediction uncertainty is assessed. Secondly, the paper focuses on the influence of the most sensitive parameters in the model. Finally, a combined analysis (particle level plus most sensitive parameters) is performed and discussed. To propagate the uncertainty originating from the parameter uncertainty to the model output, the Generalized Likelihood Uncertainty Estimation (GLUE) method is used. This method enables a modeller to incorporate the information obtained from the experimental data in the assessment of the uncertain model predictions and to find a balance between model performance and data precision. A detailed evaluation of the obtained uncertainty analysis results is made with respect to the model structure, interactions between parameters and uncertainty boundaries.
A methodology for development of biocatalytic processes

The potential advantages displayed by biocatalytic processes for organic synthesis (such as exquisite selectivity under mild operating conditions), have prompted the increasing number of processes running on a commercial scale. However, biocatalysis is still a fairly underutilised technology. As a relatively new technology biocatalytic processes often do not immediately fulfill the required process metrics that are key for an economically and/or environmentally competitive process at an industrial scale (high concentration, high reaction yield, high space-time-yield and high biocatalyst yield). These process metrics can often be attained by improvements in the reaction chemistry, the biocatalyst, and/or by process
engineering, which often requires a complex process development strategy. Interestingly this complexity, which arises from the need for integration of biological and process technologies, is also the source of the greatest opportunities. Indeed, recombinant DNA technology offers a superb complement to process technologies. Potentially this is one of the biggest advantages of biocatalysis when compared with conventional chemical catalysis, where all the reaction boundaries are fixed by the physical and thermodynamic properties of the reaction compounds. Therefore, the main avenue that still remains to be explored by process engineers is how to promote process development in a systematic way rather than on a case-by-case basis, as is frequently the case today. One of the main challenges in process development is selecting between different process alternatives. The development effort for a novel process is considerable and thus, an increasing number of conceptual process design methods are now applied in chemical industries. Since the natural environment of the biocatalyst is often very different from the operating conditions suitable for a viable process (high substrate and product concentrations, unnatural substrates, presence of organic solvents, etc.), process development strategies are particularly relevant for biocatalytic processes. However, state-of-the-art methodologies for process development applied to biocatalysis often prove to be unsuccessful. At the early development stage the biocatalysts are usually still under development and many of the reactions have not yet achieved their full potential, many of the process technologies are not yet well described and their relationship with the overall process is not clear. The work described in this thesis presents a methodological approach for early stage development of biocatalytic processes, understanding and dealing with the reaction, biocatalyst and process constraints. When applied, this methodology has a decisive role in helping to identify many of the process bottlenecks up-front and in a straightforward way, whilst indicating development targets, allowing a better use of resources and shortening development time. The methodology is illustrated through three different case studies: H-caprolactam production by a multi-enzymatic process, chiral amine production using Z-transaminase and finally long-chain chiral aliphatic Abstract ii alcohol production by a bi- enzymatic system. For each case study presented, a different tool is used to guide development and evaluate the process when different levels of underlying process knowledge are available. The first case study presents a rational approach for defining a development strategy for multi- enzymatic processes. The proposed methodology requires a profound and structured knowledge of the multi-enzyme systems, integrating chemistry, biological and process engineering. In order to suggest a reduced number of feasible process design options, cofactor and interaction matrices are used, identifying the challenges and addressing them by selecting appropriate process configurations. Based on this information, feasible flowsheets and mass and energy balances are identified. By applying evaluation tools, the number of options can be much reduced and the current process bottlenecks identified. By applying a priori this methodology, the Laboratory experts are better able to understand the most favourable operating conditions at fullscale and thus be able to collect information at these relevant conditions. In the second case study, windows of operation are used to quantify and visualise process performance and feasibility when interactions between process Technologies and biocatalyst performance (or reaction) are significant. The methodology constitutes a useful tool that provides easy interpretable results to enable rational design choices of different available process technologies. In the particular case of the asymmetric synthesis of chiral amines, the reaction constraints (thermodynamic equilibrium) must be solved prior to implementation and these fix the hard boundaries of the operating space. Improvements in the biocatalyst specific activity are also required for a successful full-scale implementation. In the third case study a methodology for bottleneck analysis is presented, incorporating process modelling and engineering evaluation tools. The benefit of such models, when integrated with evaluation tools, is that they can be used to predict the process performance and identify bottlenecks, without requiring experimental examination thereby reducing the resources and time for process development. The use of this methodology in the context of reaction engineering is to propose new operating conditions at which the process performance is improved, while identifying the remaining bottlenecks and suggesting further research efforts. Although the proposed methodology is still in its infancy when compared with other established process development methodologies, it provides a good overview of the whole reaction system and process. The proposed methodological approach establishes a systematic evaluation of different process options and indicates required fundamental data collection and development efforts for further development stages. This methodology could be greatly enhanced by the implementation and integration of in-silico tools for property and thermodynamic data as well as process mechanistic models to assist in the selection of process technologies.

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A method to estimate the enthalpy of formation of organic compounds with chemical accuracy
A model that yields chemical accuracy for a broad range of organic molecules is presented. The range of applicability of such an accurate model is very broad: it can be used by chemists to predict equilibria while fostering new chemistries and allow process engineers to make more reliable designs. The model which is group-contribution (GC) based, estimates gas phase standard enthalpy of formations (ΔfH°gas) of organic compounds. To achieve the chemical accuracy, a systematic property-data-model analysis, which allows efficient use of knowledge of the experimental data of ΔfH°gas and the molecular structural information is employed. Based on the findings of property-data-model analysis, new structural parameters are defined and included in the GC-model to provide additional structural information for compounds having large correlation errors and to thereby improve accuracy of ΔfH°gas predictions through better correlation of data. For parameter estimation, a data-set containing 861 experimentally measured values of a wide variety of organic compounds (hydrocarbons, oxygenated compounds, nitrogenated compounds, multi-functional compounds, etc.) is used. The developed property model for ΔfH°gas is fully predictive and is based exclusively on the molecular structure of the organic compound. Compared to other currently used property prediction methods, the developed GC-model for ΔfH°gas provides significant improvement in accuracy with an average absolute error of 1.75kJ/mol and standard deviation of 2.61kJ/mol.

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A model-based framework for incremental scale-up of wastewater treatment processes

Scale-up is traditionally done following specific ratios or rules of thumb which do not lead to optimal results. We present a generic framework to assist in scale-up of wastewater treatment processes based on multiscale modelling, multiobjective optimisation and a validation of the model at the new large scale. The framework is illustrated by the scale-up of a complete autotropic nitrogen removal process.

The model based multiobjective scaleup offers a promising improvement compared to the rule of thumbs based empirical scale up rules.
A Modeling Framework for Conventional and Heat Integrated Distillation Columns

In this paper, a generic, modular model framework for describing fluid separation by distillation is presented. At present, the framework is able to describe a conventional distillation column and a heat-integrated distillation column, but due to a modular structure the database can be further extended by additional configurations. The framework provides the basis for fair comparison of both steady state and dynamic performance of the different column configurations for a given binary or multicomponent separation.

A Modelling Framework for Conventional and Heat Integrated Distillation Columns

Diabatic operation of distillation columns can lead to significant reductions in energy utilization and operation cost compared to conventional (adiabatic) distillation columns, at an expense of an increased complexity of design and operation. The earliest diabatic distillation configuration dates back to the late 70s, and various different configurations have appeared since. However, at present, no full-scale diabatic distillation columns are currently operating in the industry. Current studies related to alternative distillation configurations report very different figures for potential energy savings which constitutes a problem in terms of achieving industrial acceptance. There is clearly a need for research and comparative studies which can help to provide analysis of the pros and cons of novel and intensified distillation processes compared to conventional columns for a range of separations. These studies must provide insight to both the static design properties such as the energy efficiency, utility consumption and operational cost as well as the column operability and dynamic responses to typical disturbances. Where most efforts have been directed to ideal, binary systems of close boiling mixtures of hydrocarbons such as separations of equimolar mixtures of benzene/toluene or propane/propane described by simple models, a generic, modular, model framework is presented in this work. At present, the framework is able to describe a conventional distillation column, a mechanical vapor recompression column and a heat-integrated distillation column, but due to a modular structure the database can be further extended by additional configurations. The framework provides the basis for fair comparison of both steady state and dynamic performance of the different column configurations for a given binary or multicomponent separation. Furthermore it constitutes a significant improvement in the fundamental modeling of e.g. the heat-integrated distillation column models often reported in literature and hence form a solid basis for quantitative performance evaluations.
A Multi-Scale Framework for Enterprise-Wide Design and Retrofit of Processing Networks: From Meso- to Mega-Scale

The integrated business and engineering framework for synthesis and design of process networks (Quaglia et al., 2013) developed at CAPEC allows the design of an optimal process network.

An Integrated Business and Engineering Framework for Synthesis and Design of Processing Networks

The problem of synthesis and design of processing networks corresponds to the generation, evaluation and selection among alternatives with respect to raw materials, process technologies and configurations and product portfolio compositions. This results in a complex and multi-disciplinary problem, in which all the aspects of the problem (technical, economical, regulatory, logistical, etc.) need to be considered simultaneously, in order to be able to identify the optimal design. Through the developments realized in the last decades, Process Systems Engineering has shown the potential to contribute to this problem, through the development of methods, tools, and solution approaches, under the general framework of Enterprise-Wide Optimization. Despite the level of maturity which these tools have reached and the potential which they have demonstrated, the acceptance of systematic methods and tools for synthesis and design of processing networks in the industrial sector is still lower than what could be expected. One of the key reasons for this lack of acceptance lays in their complexity. The formulation of these problems, in fact, often results in a time-consuming activity, due to the number of data that need to be gathered and of equations that need to be specified. The solution of the optimization problem formulated, moreover, requires expertise in discrete optimization, which is often not part of the standard skills set of design engineers and decision-makers. This Ph.D. project, therefore, aims at the integration of methods, tools and solution strategies for synthesis and design of processing networks in a computer-aided framework, in order to optimize and facilitate the workflow of problem formulation and solution, allowing simpler, faster and more robust use of such tools. Through the integration of different methods, tools, algorithms and databases, the framework guides the user in dealing with the mathematical complexity of the problems, allowing efficient formulation and solution of large and complex optimization problem. In this thesis, all developed methods, tools and solution strategies are described, emphasizing their integration in the computer aided framework. The framework is then applied to the formulation and solution of 3 challenging and relevant case studies, highlighting the importance of the tools integration realized in the framework.
An Intelligent System for Modelling, Design and Analysis of Chemical Processes

ICAS, Integrated Computer Aided System, is a software that consists of a number of intelligent tools, which are very suitable, among others, for computer aided modelling, sustainable design of chemical and biochemical processes, and design-analysis of product-process monitoring systems. Each of these tools are characterized by a framework that follows an established work-flow and data-flow, developed to guide the user through the many steps of the problem solution process. At each, the specific tool knows which data, model and/or algorithm to use. The tool also provides analysis of the calculated results so that the user can make intelligent decisions to proceed to the next step. The tools contain in-house databases, especially designed to work in an integrated manner with tool specific ontology for efficient knowledge management. Examples highlighting the use of the tools will be given, where the computer aided modelling tool will illustrate how to generate a desired process model, how to analyze the model equations, how to extract data and identify the model and make it ready for various types of application. In sustainable process design, the example will highlight the issue of integration of data, models and tools for consistent evaluation of sustainable process alternatives. In the case of product-process quality monitoring, the example will highlight the use of model libraries and database to analyze an existing monitoring (PAT) system.

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An Ontology for Information and Data Management for Synthesis and Design of Processing Networks

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An operational protocol for facilitating start-up of single-stage autotrophic nitrogen-removing reactors based on process stoichiometry
Start-up and operation of single-stage nitritation-anammox sequencing batch reactors (SBRs) for completely autotrophic nitrogen removal can be challenging and far from trivial. In this study, a step-wise procedure is developed based on
stoichiometric analysis of the process performance from nitrogen species measurements to systematically guide start-up and normal operation efforts (instead of trial and error). The procedure is successfully applied to laboratory-scale SBRs for start-up and maintained operation over an 8-month period. This analysis can serve as a strong decision-making tool to take appropriate actions with respect to reactor operation to accelerate start-up or ensure high-rate N removal via the nitritation–anammox pathway.

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Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.568 SNIP 0.7 CiteScore 1.3
ISI indexed (2013): ISI indexed yes
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Scopus rating (2008): SJR 0.579 SNIP 0.697
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Application of the cubic-plus-association (CPA) equation of state to model the fluid phase behaviour of binary mixtures of water and tetrahydrofuran

The complex fluid phase behaviour of the binary system comprised of water and tetrahydrofuran (THF) is modelled by use of the cubic-plus-association (CPA) equation of state. A total of seven modelling approaches are analysed, differing only in their way of describing THF and its interactions (hydrogen bonding) with water. The qualitative behaviour of the fluid phase equilibria in this system can only be described by CPA when cross-association between water and THF is allowed. Six of the seven tested modelling scenarios allow for cross-association between the two compounds. These scenarios are named Case 2 to Case 7. Case 2 treats THF as non-self-associating, but applies a single association site on the THF oxygen atom, that allows for cross-linking with a single water molecule. Case 3 is identical to Case 2 but applies two association sites on THF, allowing for simultaneous cross-association with two water molecules. Case 4 treats THF as self-associating and cross-associating according to an association scheme with two electron accepting sites and a single electron donating site. Case 5 also considers both self- and cross-association by THF, but applies an association scheme with two electron accepting- and two electron donating sites. Cases 6 and 7 are similar to Cases 4 and 5, respectively, however the binary cross-association volume between electron accepting sites on water and electron donating sites on THF is adjusted to match the CPA descriptions with available experimental VLE data. It is found that Cases 2, 3, 6 and 7 (when applying three adjustable binary parameters), are the only cases, which can describe both VLE and LLE using a single set of parameters. With a total of three binary parameters correlated to available VLE data, these data may be described with average absolute deviations of approximately 5–7 percent. The LLE is well predicted by both model Cases 2 and 3, with a slightly better phase composition prediction by Case 3. While Cases 6 and 7 describe VLE data better than the cases treating THF as solvating, the LLE is less accurately described. Based on the results presented in this work, it is suggested to model this binary system considering THF as cross-associating only, with two cross-association sites. The use of a temperature dependent binary interaction parameter and a correlated binary cross-association volume then allows for both accurate VLE and LLE descriptions in large ranges of temperature and pressure.
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Web of Science (2003): Indexed yes
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Applications, benefits and challenges of flow chemistry

Organic synthesis (incorporating both chemo-catalysis and biocatalysis) is essential for the production of a wide range of small-molecule pharmaceuticals. However, traditional production processes are mainly based on batch and semi-batch operating modes, which have disadvantages from an economic, environmental and manufacturing perspective. A potential solution to resolve these issues is to use flow chemistry in such processes, preferably with applications of micro- and mini-sized equipment. In addition, Process Analytical Technology (PAT) may be implemented in a very efficient way in such equipment due to the high degree of automation and process controllability that can be achieved in small scale continuous equipment.
Applications of Process Synthesis: Moving from Conventional Chemical Processes towards Biorefinery Processes

Concerns about diminishing petroleum reserves, enhanced worldwide demand for fuels and fluctuations in the global oil market, together with climate change and national security have promoted many initiatives for exploring alternative, non-petroleum based processes. Among these initiatives, biorefinery processes for converting biomass-derived carbohydrates into transportation fuels and chemicals are now gaining more and more attention from both academia and industry. Process synthesis, which has played a vital role for the development, design and operation of (petro) chemical processes, can be predicted to play a significant role in the design and commercialization of sustainable and cost-effective biorefinery processes. The main objective of this perspective paper is to elucidate the potential opportunities that biorenewables processing offers to optimal synthesis; challenges and future directions in this field are also concisely discussed. An attempt is made with this perspective to stimulate more and more efforts to optimally synthesize and design biorenewable conversion process to accelerate the commercialization of the biorefinery technology and further reduce the heavily reliance on petroleum-derive fuels.

General information

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Applying mechanistic models in bioprocess development.

The available knowledge on the mechanisms of a bioprocess system is central to process analytical technology. In this respect, mechanistic modeling has gained renewed attention, since a mechanistic model can provide an excellent summary of available process knowledge. Such a model therefore incorporates process-relevant input (critical process variables)-output (product concentration and product quality attributes) relations. The model therefore has great value in planning experiments, or in determining which critical process variables need to be monitored and controlled tightly. Mechanistic models should be combined with proper model analysis tools, such as uncertainty and sensitivity analysis. When assuming distributed inputs, the resulting uncertainty in the model outputs can be decomposed using sensitivity analysis to determine which input parameters are responsible for the major part of the output uncertainty. Such information can be used as guidance for experimental work; i.e., only parameters with a significant influence on model outputs need to be determined experimentally. The use of mechanistic models and model analysis tools is demonstrated in this chapter. As a practical case study, experimental data from Saccharomyces cerevisiae fermentations are used. The data are described with the well-known model of Sonnleitner and Käppeli (Biotechnol Bioeng 28:927-937, 1986) and the model is analyzed further. The methods used are generic, and can be transferred easily to other, more complex case studies as well.

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A rational approach for ω-transaminase-catalyzed process design: Synthesis of p-Br-1-phenylethylamine
Herein we describe a novel rational approach to the design of a ω-transaminase process such that it will fulfill criteria necessary for industrial use. By first determining the fundamental properties of the reaction system, it is possible to suggest appropriate process strategies that may be used to overcome any unfavorable parameters. The ω-transaminase is used as a model system because it is an important enzyme class and developing a systematic methodology would have significant value.

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Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, Dr. Reddy’s Chirotech Technology Centre
Authors: T. Gundersen, M. (Intern), Lloyd, R. (Ekstern), Tufvesson, P. (Intern), Woodley, J. (Intern)
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A_rational_approach_for_transaminase_catalyzed_process_design_synthesis_of_p_Br_1_phenylethylamine_Maria_T_Gundersen.pdf
Publication: Research - peer-review › Poster – Annual report year: 2013
A Robust Process Analytical Technology (PAT) System Design for Crystallization Processes

A generic computer-aided framework for systematic design of a process monitoring and control system for crystallization processes has been developed to study various aspects of crystallization operations. The design framework contains a generic multidimensional modelling framework, a tool for generation of the supersaturation setpoint for a supersaturation controller, a tool for design of a process monitoring and control system (also called Process Analytical Technology (PAT) system) as well as a tool for performing uncertainty and sensitivity analysis of the PAT system design. The uncertainty analysis is important in order to produce an estimate of the risk of not achieving the desired product quality with its corresponding target crystal properties.

Application of the framework is highlighted through a case study involving the design of a robust PAT system for a potassium dichromate crystallization process to achieve the target crystal size distribution (CSD) in the presence of parametric uncertainties.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Abdul Samad, N. A. F. B. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Number of pages: 8
Publication date: 2013

A systematic framework for design of process monitoring and control (PAT) systems for crystallization processes

A generic computer-aided framework for systematic design of a process monitoring and control system for crystallization processes has been developed to study various aspects of crystallization operations. The systematic design framework contains a generic crystallizer modelling toolbox, a tool for generation of the supersaturation set-point for supersaturation control, as well as a tool for design of a process monitoring and control system (also called Process Analytical Technology (PAT) system). This systematic design allows one to generate the necessary problem-chemical system specific model, the necessary supersaturation set-point as well as a PAT system design including implementation of monitoring tools and control strategies in order to produce the desired target product properties notably crystal size distribution (CSD) and shape for a wide range of crystallization processes. Application of the framework is highlighted through a case study involving the design of a monitoring and control system for a potassium dihydrogen phosphate (KDP) crystallization process, where also the one-dimensional CSD and two-dimensional CSD modelling features are highlighted.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Abdul Samad, N. A. F. B. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
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Main Research Area: Technical/natural sciences

Publication information
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BFI (2017): BFI-level 2
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Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
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A Systematic Framework for Design of Process Monitoring and Control (PAT) Systems for Crystallization Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Environmental Engineering, Center for Process Engineering and Technology

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
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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
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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 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
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Crystallization, Generic modelling framework, Analytical CSD estimator, Response surface method, PAT system

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A systematic framework for enterprise-wide optimization: Synthesis and design of processing network under uncertainty

In this paper, a systematic framework for synthesis and design of processing networks under uncertainty is presented. Through the framework, an enterprise-wide optimization problem is formulated and solved under uncertain conditions, to identify the network (composed of raw materials, process technologies and product portfolio) which is feasible and have optimal performances over the entire uncertainty domain. Through the integration of different methods, tools, algorithms and databases, the framework guides the user in dealing with the mathematical complexity of the problems, allowing efficient formulation and solution of large and complex enterprise-wide optimization problem. Tools for the analysis of the uncertainty, of its consequences on the decision-making process and for the identification of strategies to mitigate its impact on network performances are integrated in the framework. A decomposition-based approach is employed to deal with the added complexity of the optimization under uncertainty. A network benchmarking problem is proposed as a benchmark for further development of methods, tools and solution approaches. To highlight the features of the framework, a large industrial case study dealing with soybean processing is formulated and solved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 47-62
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Main Research Area: Technical/natural sciences
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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
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI 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
A Tool to Support Optimal Industrial Wastewater Treatment Design and Analysis

Industrial Wastewater Treatment Plant (IWWTP) design is often based on in-house expert knowledge and experience. Because of time and resources constraints, only a small number of alternative treatment configurations and ideas are evaluated while designing an IWWTP. Consequently, the selected design may be suboptimal or disregard opportunities for water recycle or resource recovery and reuse. In this contribution, we propose a model-based toolbox developed to help wastewater professionals to screen among a large number of alternatives in order to identify the optimal treatment configuration from an economic cost-benefit perspective. The toolbox is demonstrated through a case study, dealing with oil refinery wastewater treatment and water recycle.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
Authors: Quaglia, A. (Intern), Pennati, A. (Ekstern), Bozkurt, H. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Publication date: 2013
Event: Main Research Area: Technical/natural sciences
Industrial wastewater treatment, Water reuse and recycle, Refinery wastewater, Design and optimization
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013
A Tuning Procedure for ARX-based MPC

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for univariate processes that can be represented by an ARX model. The advantage of ARX model representations is that standard system identification techniques using convex optimization can be used for identification of such models from input-output data. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The ARMAX model description resulting from the extension can be realized as a state space model in innovation form. The MPC is designed and implemented based on this state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop expressions, these evaluations can be done relative quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, Scientific Computing
Authors: Olesen, D. (Intern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
Pages: 188-193
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A Tuning Procedure for ARX-based MPC of Multivariate Processes

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for multivariate processes that can be represented by an ARX model. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The MPC is designed and implemented based on a state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop expressions these evaluations can be done relative quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure. The method is demonstrated for two simulated examples: A Wood-Berry distillation column example and a cement mill example.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, Scientific Computing
Authors: Olesen, D. (Intern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
Pages: 1721-1726
Publication date: 2013

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Benchmark simulation models, quo vadis?
As the work of the IWA Task Group on Benchmarking of Control Strategies for wastewater treatment plants (WWTPs) is coming to an end, it is essential to disseminate the knowledge gained. For this reason, all authors of the IWA Scientific and Technical Report on benchmarking have come together to provide their insights, highlighting areas where knowledge may still be deficient and where new opportunities are emerging, and to propose potential avenues for future development and application of the general benchmarking framework and its associated tools. The paper focuses on the topics of temporal and spatial extension, process modifications within the WWTP, the realism of models, control strategy extensions and the potential for new evaluation tools within the existing benchmark system. We find that there are major opportunities for application within all of these areas, either from existing work already being done within the context of the benchmarking simulation models (BSMs) or applicable work in the wider literature. Of key importance is increasing capability, usability and transparency of the BSM package while avoiding unnecessary complexity. © IWA Publishing 2013.
Biokatalysatorens vej til industrien

Gernadey, K. (Intern), Woodley, J. (Intern)

Computer simulation, Control, Models, Process monitoring, Tools, Wastewater treatment, Benchmarking

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Authors: Krühne, U. (Intern), Heintz, S. (Intern), Pereira Rosinha, I. (Intern), Ringborg, R. H. (Intern), Tufvesson, P. (Intern)
, Gernaey, K. (Intern), Woodley, J. (Intern)

Pages: 18-22
Publication date: 2013
Main Research Area: Technical/natural sciences
Calibration and validation of a model describing complete autotrophic nitrogen removal in a granular SBR system

BACKGROUND: A validated model describing the nitritation-anammox process in a granular sequencing batch reactor (SBR) system is an important tool for: a) design of future experiments and b) prediction of process performance during optimization, while applying process control, or during system scale-up. RESULTS: A model was calibrated using a step-wise procedure customized for the specific needs of the system. The important steps in the procedure were initialization, steady-state and dynamic calibration, and validation. A fast and effective initialization approach was developed to approximate pseudo steady-state in the biofilm system. For oxygen mass transfer coefficient (kLa) estimation, long-term data, removal efficiencies, and the stoichiometry of the reactions were used. For the dynamic calibration a pragmatic model fitting approach was used - in this case an iterative Monte Carlo based screening of the parameter space proposed by Sin et al. (2008) - to find the best fit of the model to dynamic data. Finally, the calibrated model was validated with an independent data set. CONCLUSION: The presented calibration procedure is the first customized procedure for this type of system and is expected to contribute to achieve a fast and effective model calibration, an important enabling tool for various biochemical engineering design, control and operation problems.
Capec Consortium: Effective Academic-Industrial Interactions Strengthened By Surveys and Analyses of Gaps in Properties Modeling

The CAPEC Consortium has operated for many years. Starting with UNIFAC correlations for activity coefficients, the research has branched out to many other properties like critical properties, heats of formation, boiling points, heats of vaporization, and many others.

One key to CAPEC's success has been the establishment of an industrial advisory committee at an early stage. This committee meets annually to provide guidance about which properties are of top priority for the coming year(s). This process will be reviewed along with the resulting compilation of properties of interest and its evolution with time. One key to CAPEC's success has been the establishment of an industrial advisory committee at an early stage. This committee meets annually to provide guidance about which properties are of top priority for the coming year(s). This process will be reviewed along with the resulting compilation of properties of interest and its evolution with time.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, University of Virginia
Authors: O'Connell, J. P. (Ekstern), Gani, R. (Intern)
Cell mass and cell cycle dynamics of an asynchronous budding yeast population: Experimental observations, flow cytometry data analysis, and multi-scale modeling

Despite traditionally regarded as identical, cells in a microbial cultivation present a distribution of phenotypic traits, forming a heterogeneous cell population. Moreover, the degree of heterogeneity is notably enhanced by changes in micro-environmental conditions. A major development in experimental single-cell studies has taken place in the last decades. It has however not been fully accompanied by similar contributions within data analysis and mathematical modeling. Indeed, literature reporting, for example, quantitative analyses of experimental single-cell observations and validation of model predictions for cell property distributions against experimental data is scarce. This study focuses on the experimental and mathematical description of the dynamics of cell size and cell cycle position distributions, of a population of Saccharomyces cerevisiae, in response to the substrate consumption observed during batch cultivation. The good agreement between the proposed multi-scale model (a population balance model [PBM] coupled to an unstructured model) and experimental data (both the overall physiology and cell size and cell cycle distributions) indicates that a mechanistic model is a suitable tool for describing the microbial population dynamics in a bioreactor. This study therefore contributes towards the understanding of the development of heterogeneous populations during microbial cultivations. More generally, it consists of a step towards a paradigm change in the study and description of cell cultivations, where average cell behaviors observed experimentally now are interpreted as a potential joint result of various co-existing single-cell behaviors, rather than a unique response common to all cells in the cultivation.
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
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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
Scopus rating (1999): SJR 1.511 SNIP 1.567

Original language: English
Population balance model (PBM), Multiscale modeling, Flow cytometry, Standardized data analysis, Saccharomyces cerevisiae, Total protein content, Cell cycle

DOIs:
10.1002/bit.24749
Computer-Aided Modeling Framework: A Generic Template as a Modeling Tool

Models are playing important roles in design and analysis of chemicals based products and the processes that manufacture them. Computer-aided methods and tools have the potential to reduce the number of experiments, which can be expensive and time consuming, and there is a benefit of working with them. As the required models may be complex and require multiple time and/or length scales, their development and application for product-process design is not trivial. Therefore, a systematic modeling framework can contribute by significantly reducing the time and resources needed for model development and application. The proposed work is a part of the project for development of methods and tools that will allow systematic generation, analysis and solution of models for various objectives. It will use the computer-aided modeling framework that is based on a modeling methodology, which combines in-depth work-flows and data-flows for different modeling tasks related to model development and application with the goal to systematize the modeling. The overall objective of this work is to allow the model developer to generate and test models systematically, efficiently and reliably. In this contribution, the concept of template-based modeling is presented and application is highlighted for the specific case of catalytic membrane fixed bed models. The modeling template is integrated in a generic computer-aided modeling framework. Furthermore, modeling templates enable the idea of model reuse as the user can then generate many problem-specific models for different applications. The templates are part of the model generation feature of the framework. Also, the model development and use for a product performance evaluation has been developed. The application of the modeling template is highlighted with a case study related to the modeling of a catalytic membrane reactor coupling dehydrogenation of ethylbenzene with hydrogenation of nitrobenzene, and, for the performance evaluation of an atomizer product. In the first case study, the reactor type is where the reactions are thermodynamically limited, such as, steam reforming and the production of olefins from inexpensive paraffins via dehydrogenation. The generated process model is based on Fickian diffusion model, which is the most widely used to account for the intraparticle mass transfer resistance. The model of the process can help to predict the yield and the quality of the output components and that will make possible to evaluate and improve the product properties. In the case of the atomizer performance, the droplet size, number and their evaporation are analyzed through a multiscale model. The mathematical equations of the model are generated through the template in ICAS-MoT and translated into a model object. Once in ICAS-MoT, the model is numerical analyzed, solved and identified. A computer-aided modeling framework integrating systematic model derivation and development tools has been developed. It includes features for model development, model identification and solution, model templates library. In this work the template based model application feature was extended with a modeling template related for catalytic membrane fixed bed reactor and a template related for product performance evaluation.

General information
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Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Main Research Area: Technical/natural sciences

Computer-aided modeling framework: a generic template as a modeling tool
This work focuses on the development of a computer-aided modeling framework. The framework is a knowledge-based system that is built on a generic modeling language and structured on workflows for different modeling tasks. The overall objective is to support model developers and users to generate and test models systematically, efficiently and reliably. In this way, development of products and processes can be made faster, cheaper and more efficient. In this contribution, as part of the framework, a generic modeling template for the systematic derivation of problem specific models is presented. The application of the modeling template is highlighted with a case study related to the modeling of a catalytic membrane reactor coupling dehydrogenation of ethylbenzene with hydrogenation of nitrobenzene.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Computer-aided modeling framework – a generic modeling template for catalytic membrane fixed bed reactors
This work focuses on development of computer-aided modeling framework. The framework is a knowledge-based system that is built on a generic modeling language and structured based on workflows for different general modeling tasks. The overall objective of this work is to support the model developers and users to generate and test models systematically, efficiently and reliably. In this way, development of products and processes can be faster, cheaper and very efficient.
In this contribution, as part of the framework a generic modeling template for the systematic derivation of problem specific catalytic membrane fixed bed models is developed. The application of the modeling template is highlighted with a case study related to the modeling of a catalytic membrane reactor coupling dehydrogenation of ethylbenzene with hydrogenation of nitrobenzene.

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Modeling framework, Fixed bed reactor, Computer-aided modeling.
Source: dtu
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

Computer-Aided Solvent Screening for Biocatalysis
A computer-aided solvent screening methodology is described and tested for biocatalytic systems composed of enzyme, essential water and substrates/products dissolved in a solvent medium, without cells. The methodology is computationally simple, using group contribution methods for calculating constrained properties related to chemical reaction equilibrium, substrate and product solubility, water solubility, boiling points, toxicity and others. Two examples are provided, covering the screening of solvents for lipase-catalyzed transesterification of octanol and inulin with vinyl laurate. Esterification of acrylic acid with octanol is also addressed. Solvents are screened and candidates identified, confirming existing experimental results. Although the examples involve lipases, the method is quite general, so there seems to be no preclusion against application to other biocatalysts.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Wageningen University & Research
Authors: Abildskov, J. (Intern), Leeuwen, M. V. (Ekstern), Boeriu, C. (Ekstern), Broek, L. V. D. (Ekstern)
Pages: 200-213
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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
Computer aided solvent selection, design and application

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Considerations for a methodology for selection of cascades for co-product removal in \( \omega \)-transaminase systems

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Janes, K. (Intern), Gernaey, K. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Publication date: 2013
Event: Abstract from BIOTRANS 2013, Manchester, United Kingdom.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Control assessment for heat integrated systems. An industrial case study for ethanol recovery

Heat integration is essential for reducing the energy consumption of process industries. However, it may render the dynamic operation more interactive and difficult to control. This paper assesses the implications of heat integration in controllability and performance in energy reduction. The assessment, both on open loop and closed loop, was carried out based on an industrial case study and compared to a modified case without heat integration. Although the heat integrated system displayed a certain deterioration of controllability, the control system made possible an efficient operation. To this goal, different control systems were tested, from a decentralized control system to a model predictive controller. The type of controller used in the process barely influenced the performance of the process since the aim was exclusively to ensure the regulation of the process to fixed setpoints. The reduction of energy consumption achieved thanks to heat integration was considerably larger than the losses due to poor control of the process, confirming the importance of heat integration in energy intensive processes.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mauricio Iglesias, M. (Intern), Huusom, J. K. (Intern), Sin, G. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.766 SNIP 1.205 CiteScore 2.57
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.837 SNIP 1.389 CiteScore 2.63
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.87 SNIP 1.427 CiteScore 2.41
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.972 SNIP 1.391 CiteScore 2.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Control of a Biological Nitrogen Removal Process in an Intensified Single Reactor Configuration

The nitrogen removing granular sludge process is a novel and intensified process. However, its stable operation and control remains a challenging problem. In this contribution, a new process oriented approach is used to develop, evaluate and benchmark control strategies to ensure stable operation and rejection of disturbances. Three control strategies were developed: a feedforward control (case 1), a rule-based feedback control (case 2), and a feedforward-feedback controller, in which the feedback loop updates the set point of the feedforward loop (case 3). The case 1 controller, based on influent measurements, was giving the best performance against disturbances in the ammonium concentration, whereas case 2 was providing the best performance against disturbances in the organic carbon concentration. The case 3 controller rejected both disturbances satisfactorily. Thus, this controller provided versatility towards disturbance rejection, however through a less tight control, which meant a bigger offset from the removal efficiency.
Control of a Biological Nitrogen Removal Process in an Intensified Single Reactor Configuration

The nitrogen removing granular sludge process is a novel and intensified process. However, its stable operation and control remains a challenging problem. In this contribution, a new process oriented approach is used to develop, evaluate and benchmark control strategies to ensure stable operation and rejection of disturbances. Three control strategies were developed: a feedforward control (case 1), a rule-based feedback control (case 2), and a feedforward-feedback controller, in which the feedback loop updates the set point of the feedforward loop (case 3). The case 1 controller, based on influent measurements, showed the best performance against disturbances in the ammonium concentration, whereas case 2 was providing the best performance against disturbances in the organic carbon concentration. The case 3 controller rejected both disturbances satisfactorily. Thus, this controller provided versatility towards disturbance rejection, however through a less tight control, which meant a larger offset from the desired removal efficiency.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Vangsgaard, A. K. (Intern), Mauricio Iglesias, M. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Publication date: 2013
Control of a Novel Energy Efficient Biological Nitrogen Removal Process

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Vangsgaard, A. K. (Intern), Mauricio Iglesias, M. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
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Control system design for the wastewater system: The different approaches and their advantages and disadvantages

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Environmental Engineering, Urban Water Engineering, Copenhagen Wastewater Innovation and Copenhagen Energy
Authors: Mollerup, A. L. (Intern), Mikkelsen, P. S. (Intern), Johansen, N. B. (Ekstern), Thornberg, D. (Ekstern), Sin, G. (Intern)
Number of pages: 22
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Original language: English
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Sound/Visual production (digital) – Annual report year: 2013

Crystallization Kinetics within a Generic Modelling Framework
An existing generic modelling framework has been expanded with tools for kinetic model analysis. The analysis of kinetics is carried out within the framework where kinetic constitutive models are collected, analysed and utilized for the simulation of crystallization operations. A modelling procedure is proposed to gain the information of crystallization operation kinetic model analysis and utilize this for faster evaluation of crystallization operations.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Center for Process Engineering and Technology
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Source-ID: u::9395
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Data, analysis and modeling of physical properties for process designof systems involving lipids
Pure component and mixture properties are necessary for synthesis, design, and analysis of processes for the production of edible oils, fats, biodiesel, and other lipids. The lack of measured data for these systems makes it necessary to develop reliable predictive models based on limited data. We have systematically collected data for vapor–liquid equilibrium (VLE), solid–liquid equilibrium (SLE) and related pure component properties involving lipid systems as a first step toward developing relevant property models. The established consistency tests to evaluate the VLE data of lipid systems as well
as lipid properties are briefly reviewed. For SLE systems, where consistency tests based on the Gibbs–Duhem equation cannot be implemented, a consistency test has been developed. It involves limiting conditions and regression of the parameters for a new thermodynamic model that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions. This model gives noticeably better descriptions of experimental data in lipid systems than do traditional models. Examination of various objective functions for regressing model parameters showed that some variation of parameter values and differences in accuracy can be found, though they are not large. Some original UNIFAC group contribution parameters for lipids have been revised by fitting to the lipid database.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, State University of Campinas, Alfa Laval Copenhagen A/S, University of Virginia
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- 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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- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
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- Web of Science (2011): Indexed yes
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- Web of Science (2009): Indexed yes
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Data, analysis, modeling, and prediction of properties and phase equilibria for process design of edible oil and biodiesel systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S, University of Virginia, State University of Campinas
Authors: Cunico, L. (Intern), Ceriani, R. (Ekstern), Sarup, B. (Ekstern), O’Connell, J. P. (Ekstern), Gani, R. (Intern)
Number of pages: 1
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Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Journal article – Annual report year: 2013

Denmark’s Chemicals Industry: Progress and Challenges

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre
Authors: Sin, G. (Intern), Gani, R. (Intern), Dam-Johansen, K. (Intern)
Pages: 54-59
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): SJR 0.165 SNIP 0.188 CiteScore 0.33
Designing Robust Process Analytical Technology (PAT) Systems for Crystallization Processes: A Potassium Dichromate Crystallization Case Study

The objective of this study is to test and validate a Process Analytical Technology (PAT) system design on a potassium dichromate crystallization process in the presence of input uncertainties using uncertainty and sensitivity analysis. To this end a systematic framework for managing uncertainties in PAT system design is used. For uncertainty analysis the Monte Carlo technique is used, while for the sensitivity analysis both Standardized Regression Coefficients (SRC) and Morris methods are employed. The analysis performed under open-loop condition shows that the input uncertainties in the nucleation and crystal growth parameters affect the product-process performances (e.g. crystal size distribution (CSD)). Analysis of the proposed PAT system design (closed-loop), on the other hand, shows that the effect of the input uncertainties on the outputs (product quality) is minimized, and the target specifications are achieved, thus ensuring that the PAT system design is reliable under the considered uncertainty ranges.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Abdul Samad, N. A. F. B. (Intern), Sin, G. (Intern)
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Main Research Area: Technical/natural sciences
Design methodology for bio-based processing: Biodiesel and fatty alcohol production
A systematic design methodology is developed for producing multiple main products plus side products starting with one or more bio-based renewable source. A superstructure that includes all possible reaction and separation operations is generated through thermodynamic insights and available data. The number of alternative processes is systematically reduced through a screening procedure until only feasible alternatives are obtained. As part of the methodology, process intensification involving reaction-separation tasks is also considered to improve the design by shifting the equilibrium reactions. Economic analysis and net present value are determined to find the best economically and operationally feasible process. The application of the methodology is presented through a case study involving biodiesel and fatty alcohol productions.
Design of a Generic and Flexible Data Structure for Efficient Formulation of Large Scale Network Problems

The formulation of Enterprise-Wide Optimization (EWO) problems as mixed integer nonlinear programming requires collecting, consolidating and systematizing large amount of data, coming from different sources and specific to different disciplines. In this manuscript, a generic and flexible data structure for efficient formulation of enterprise-wide optimization problems is presented. Through the integration of the described data structure in our synthesis and design framework, the problem formulation workflow is automated in a software tool, reducing time and resources needed to formulate large problems, while ensuring at the same time data consistency and quality at the application stage.

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
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Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology

An extended systematic methodology for the design of emulsion-based Chemical products is presented. The methodology consists of a model-based framework involving seven sequential hierarchical steps: starting with the identification of the needs to be satisfied by the product and then adding one-by-one the different classes of chemicals, until a formulation is obtained, the stability of which as an emulsion is finally checked with appropriate models. Structured databases, appropriate pure component as well as mixture property models, rule-based selection criteria and CAMD techniques are employed together to obtain one or more candidate formulations. A conceptual casestudy representing a personal detergent is presented to highlight the methodology.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Columbia University
Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
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Design of future municipal wastewater treatment plants: A mathematical approach to manage complexity and identify optimal solutions

The increasing number of alternative wastewater treatment (WWT) technologies and stricter effluent requirements imposed by regulations make the early stage decision making for WWTP layout design, which is currently based on expert decisions and previous experiences, much harder. This paper therefore proposes a new approach based on mathematical programming to manage the complexity of the problem and generate/identify novel and optimal WWTP layouts for municipal/domestic wastewater treatment. Towards this end, after developing a database consisting of primary, secondary and tertiary WWT technologies to build a superstructure, the design problem was formulated as a Mixed Integer Nonlinear Programming problem (MINLP). The tool generates many process alternatives and evaluates them with respect to their optimality. The objective function minimizes the operation cost. The design problem is thus solved to obtain the optimal WWT network and the optimal wastewater and sludge flow through the network. The tool is evaluated on a case study, which was chosen as the Benchmark Simulation Model no.1 (BSM1) and many retrofitting options for obtaining a cost-effective treatment were investigated with the help of the tool. The resulting solutions to the optimization problem are discussed in detail.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology

Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology

General information
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Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
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Design of future municipal wastewater treatment plants: A mathematical approach to manage complexity and identify optimal solutions

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Design of sustainable blended products using an integrated methodology

This paper presents a systematic methodology for designing blended products consisting of three stages: product design, process identification and experimental verification. The product design stage is considered in this paper. The objective of this stage is to screen and select suitable chemicals to be used as building blocks in the mixture design, and then to propose the blend formulations that fulfill the desired product attributes. The result is a set of blends that match the constraints, the compositions, values of the target properties and information about their miscibility. The methodology has been applied to design several blended products. A case study on design of blended lubricants is highlighted. The objective is to identify blended products that satisfy the product attributes with at least similar or better performance compared to conventional products.

Design of Sustainable Blended Products using an Integrated Methodology
This paper presents a systematic methodology for designing blended products consisting of three stages: product design, process identification and experimental verification. The product design stage is considered in this paper. The objective of this stage is to screen and select suitable chemicals to be used as building blocks in the mixture design, and then to propose the blend formulations that fulfill the desired product attributes. The result is a set of blends that match the constraints, the compositions, values of the target properties and information about their miscibility. The methodology has been applied to design several blended products. A case study on design of blended lubricants is highlighted. The objective is to identify blended products that satisfy the product attributes with at least similar or better performance compared to conventional products.

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Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology

Commercial and industrial detergents, formulated liquid blends, have recently become extremely sophisticated, in order to address a broad range of cleaning tasks and to deliver superior performances with a minimum of effort and time. These products, by definition, consist of different chemicals, each with a specific function related to the needs of the product: surfactants, builders, bleaching agents, enzymes and minors, usually mixed together with a carrier, necessary to keep the blend as a homogeneous liquid formulation. A system approach and associated tools can help to virtually generate and test different candidates in order to identify the most promising formulations before a detailed experimental stage for final selection and product development is applied. In this way, the whole design procedure speeds up, saving time and money, and the optimum formulation is identified, since a broad range of alternatives are investigated. The approach adopted for the design of emulsion-based chemical products consists in a systematic model-based methodology employing seven hierarchical steps: starting with the identification of the product needs and their translation into appropriate target properties, then building the formulation by adding, one-by-one, the different classes of chemicals needed for each function: from the active ingredients, to the solvents, the emulsifier and the additives, and finally determining the optimal composition of the formulated product. The design of the ingredients, driven by selection criteria based on the functional properties of each category of chemicals as well as by consideration of effectiveness, safety, toxicity and cost, is done through a data-model based computer aided molecular design technique. When a model-based design is not applicable since the functional properties needed to perform a rigorous choice are not readily available for consideration in a product design methodology, rule-based selection criteria are applied. These are centered on structured databases, where some relevant properties (e.g. safety or toxicity-related), if not available, are predicted through dedicated pure component property models. Once all the most advantageous ingredients have been chosen, the recipe candidates are identified through a knowledge-based mixture design method, where economic considerations are included together with appropriate boundaries related to solubility, stability, toxicity and safety issues. A special database of chemicals, classified according to their function and associated properties, has been developed. Also, a model library consisting of pure component and mixture property models has been developed so that the needed functional properties can be reliably predicted when their data cannot be found in the database. The abovementioned methodology and related tools are generic, in the sense that many different emulsified products can be designed through this framework once the needs-property relations are established, and they are here highlighted through a case-study dealing with the design of a tank cleaning blend. The main focus of this contribution is on the design of surfactants, primary responsible for the cleaning activity, thanks to a comprehensive framework based on newly developed both pure component and mixture property models. The workflow methodology with associated models, tools, databases and algorithms will be implemented into a computer-aided framework for emulsion-based formulation design.

General information
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Publication date: 2013
Main Research Area: Technical/natural sciences

Relations
Activities:
Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology
Development and Analysis of Group Contribution Plus Models for Property Prediction of Organic Chemical Systems
Prediction of properties is important in chemical process-product design. Reliable property models are needed for increasingly complex and wider range of chemicals. Group-contribution methods
provide useful tool but there is a need to validate them and improve their accuracy when complex chemicals are present in the mixtures. In accordance with that, a combined group-contribution and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties. This so-called Group- ContributionPlus (GCPlus) approach is a hybrid model which combines group contribution and molecular descriptor theories (such as connectivity indices – CI). Connectivity indices are formalisms defined via graph theoretical concepts intended to describe the topological characteristics of molecular structures. The main idea is the use of connectivity indices to describe the molecular fragmentation that relates properties which is the molecular interactions with the molecular structures. One well known and established group-contribution method is the UNIFAC model, used to predict liquid phase activity coefficients for mixtures. The needed values of the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are, however many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, which may not be feasible, values of the missing GIPs, can be predicted through the GCPlus approach. The predicted values for the GIPs are then used in the UNIFAC model to calculate activity coefficients. This approach can increase the application range of any “host” UNIFAC model by providing a reliable predictive model towards fast and efficient product development.

This PhD project is focused on the analysis and further development of the GCPlus approach for predicting mixture properties to be called the UNIFAC-CI model. The contributions of this work include an analysis of the developed Original UNIFAC-CI model in order to investigate why the model does not perform as well as the reference UNIFAC model for some systems while performing surprisingly better than the reference model for other systems. In this analysis, it is found that by introducing more structural information to the CHO group through the valence connectivity index (CI), the correlation error involving alkanes-aldehydes system can be reduced. This work is presented in Chapter 3. Furthermore in Chapter 4, as a continuation of the analysis done for systems involving C, H and O atoms, the Original UNIFAC-CI (VLE) model has been further reused and significantly expanded by including nitrogenated, chlorinated and sulfuratated systems and the involved atom interaction parameters (AIPs) have been regressed. In addition to that, another set of parameters have been generated for the Original UNIFAC-CI (VLE) model using a quality assessment algorithm, QVLE (combination of 4 VLE consistency tests) as a weighting factor for each VLE dataset in the objective function for regression of AIPs. The quality factors are useful in identifying anomalous systems which can be problematic in the parameter estimation and can produce parameters which are not accurately representing the systems used for the regression. Moreover, in Chapter 5 the Original UNIFAC-CI (VLE/SLE) model have been developed where the atom interaction parameters (AIPs) are obtained through regression against both VLE and SLE experimental data. The prediction accuracy of SLE systems using the regressed parameters has been slightly increased. Besides that, in Chapter 6, Modified (Dortmund) UNIFAC-CI has been further developed by including chlorinated and sulfuratated VLE systems. Finally, in Chapter 7, the developed Original UNIFAC-CI (VLE/SLE) model have been highlighted in selected case studies involving the design of a working solution for hydrogen peroxide production and solubility investigation of pharmaceutical systems where new group have been created and their interaction parameters are predicted/fine tuned generating a master parameter table specifically for those case studies. Also, the applicability of the Original UNIFACCI model is shown for predicting phase equilibria of lipid systems, filling missing GIPs and improving prediction of azeotropic mixture. In Chapter 8, a discussion with concluding remarks and recommendation for future work are presented.
Development of a Population Balance Model of a Pharmaceutical Drying Process and Testing of Solution Methods

Drying is frequently used in the production of pharmaceutical tablets. Simulation-based control strategy development for such a drying process requires a detailed model. First, the drying of wet granules is modelled using a Population Balance Model. A growth term based on a reduced model was used, which describes the decrease of the moisture content, to follow the moisture content distribution for a batch of granules. Secondly, different solution methods for solving the PBM are compared. The effect of grid size (discretization methods) is analyzed in terms of accuracy and calculation time. All tested methods are compared based on their ability to predict moment dynamics and the distribution, and their computational burden. The Method of Characteristics, a fast method, is able to calculate the distribution accurately with a coarse grid. The Quadrature Method of Moments requires even less calculation time, but results in a set of moments. © 2012 Elsevier Ltd.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Ghent University
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Web of Science (2016): Indexed yes
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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Development of pure component property models for chemical product-process design and analysis

Property prediction models based on the group-contribution+ (GC+) approach have been developed to provide reliable predictions of pure component properties together with uncertainties of predicted property values which is much needed information in performing chemical product and process design and analysis of sustainable chemical processes. For developing property models, a systematic methodology for property modeling and uncertainty analysis is employed. The methodology includes a parameter estimation step to determine parameters of the property model and an uncertainty analysis step to establish statistical information about the quality of parameter estimation, such as the parameter covariance, the standard errors in predicted properties, and the confidence intervals. For parameter estimation, large data sets of experimentally measured property values of a wide range of pure components taken from the CAPEC database, the US Environmental Protection Agency (EPA) database, and the USEtox database are used. In total, 21 thermo-physical properties and 22 environmental-related properties of pure components which include normal boiling point, critical constants, standard enthalpy of formation, liquid viscosity, fathead minnow 96-h LC50, oral rat LD50, global warming potential, emission to urban air (carcinogenic and noncarcinogenic) among others are modeled and analyzed. For all the estimated pure component properties, the corresponding 95% confidence intervals are also reported thereby providing information on the degree of accuracy of the property estimates. In addition, a method based on the ‘molecular structural similarity criteria’ is developed so that efficient use of knowledge of properties could be made in the development/improvement of property models. This method, in principle, can be applied to a wide range of properties of pure components. In this work, however, the application of ‘molecular structural similarity criteria’ is illustrated by considering performance improvement of models for enthalpy of formation, enthalpy of fusion, and critical temperature. For all properties listed above, it has been possible to achieve significant improvements in the performance of their models. The improved GC model for enthalpy of formation yields an average absolute deviation of 1.75 kJ/mol, which is well within the required chemical accuracy. Important issues related to property modeling such as: (i) quantity of property data used for the parameter regression; (ii) selection of the most appropriate form of the property model function; and (iii) the accuracy and thermodynamic consistency of predicted property values are also discussed. The developed models have been implemented into ProPred®, a property estimation toolbox of Integrated Computer Aided System, ICAS®, developed at CAPEC, DTU. Finally, a methodology for performing sensitivity analysis of process design due to uncertainties of property estimates is presented. This methodology allows the user to evaluate the effects of uncertainties of property estimates on
the final design; list and rank properties that are most important from process design point of view; and establish acceptable levels of accuracy for property models. The application of this methodology is highlighted through three case studies namely, design of an extractive distillation process, design of a short-path evaporator, and design of a de-acidification system of vegetable oil deodorization process.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
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Driving towards stratified aggregation in single-stage nitritation/anammox reactors by varying aeration regimes

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Publication: Research - peer-review › Poster – Annual report year: 2013

Dynamic effects of diabatization in distillation columns

The dynamic effects of diabatization in distillation columns are investigated in simulation emphasizing the heat-integrated distillation column (HIDiC). A generic, dynamic, first-principle model has been formulated, which is flexible enough to describe various diabatic distillation configurations. Dynamic Relative Gain Array and Singular Value Analysis have been applied in a comparative study of a conventional distillation column and a HIDiC. The study showed increased input-output coupling due to diabatization. Feasible SISO control structures for the HIDiC were also found and control-loop feasibility was demonstrated.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Bisgaard, T. (Intern), Huusom, J. K. (Intern), Abildskov, J. (Intern)
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Fluid separations, Distillation columns, Diabatic distillation, Dynamic modeling
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Dynamic effects of diabatization in distillation columns

General information
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Dynamic modeling and validation of a lignocellulosic enzymatic hydrolysis process: A demonstration scale study

The enzymatic hydrolysis process is one of the key steps in second generation biofuel production. After being thermally pretreated, the lignocellulosic material is liquefied by enzymes prior to fermentation. The scope of this paper is to evaluate a dynamic model of the hydrolysis process on a demonstration scale reactor. The following novel features are included: the application of the Convection–Diffusion–Reaction equation to a hydrolysis reactor to assess transport and mixing effects; the extension of a competitive kinetic model with enzymatic pH dependency and hemicellulose hydrolysis; a comprehensive pH model; and viscosity estimations during the course of reaction. The model is evaluated against real data extracted from a demonstration scale biorefinery throughout several days of operation. All measurements are within predictions uncertainty and, therefore, the model constitutes a valuable tool to support process optimization, performance monitoring, diagnosis and process control at full-scale studies.

General information
State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Prunescu, R. M. (Intern), Sin, G. (Intern)
Pages: 393–403
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Scopus rating (2014): SJR 2.41 SNIP 2.104 CiteScore 5.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.412 SNIP 2.503 CiteScore 5.97
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 2.389 SNIP 2.465 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Early stage design and analysis of biorefinery networks

Recent work regarding biorefineries resulted in many competing concepts and technologies for conversion of renewable bio-based feedstock into many promising products including fuels, chemicals, materials, etc. The design of a biorefinery process requires, at its earlier stages, the selection of the process configuration which exhibits the best performances, for a given set of economical, technical and environmental criteria. To this end, we formulate a computer-aided framework as an enabling technology for early stage design and analysis of biorefineries. The tool represents different raw materials, different products and different available technologies and proposes a conceptual (early stage) biorefinery network. This network can then be the basis for further detailed and rigorous model-based studies. In this talk, we demonstrate the application of the tool for generating an early stage optimal biorefinery concept for a lignocellulosic biorefinery. More specifically we highlight the required information management (management of various sources of data), the superstructure which is needed to represent the design space, generic but simple models covering all the processing steps of biorefineries, and the formulation and solution of an MINLP problem to identify the optimal processing route for multiple raw materials and products. Finally, economic, sustainability and LCA analysis are performed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Sin, G. (Intern)
Publication date: 2013
Event:
Main Research Area: Technical/natural sciences
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Editorial note for the 2011 Computers & Chemical Engineering Best Paper Award

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Columbia University
Authors: Gani, R. (Intern), Venkatasubramanian, V. (Ekstern)
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BFI (2011): BFI-level 2
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ISI indexed (2011): ISI indexed yes
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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
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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
**Effect of critical process parameters on the synthesis of chiral amines**

Developing a biocatalytic transferase process involves many challenges, and choices have to be made regarding several aspects. Primarily, the selection of the biocatalyst itself and which biocatalyst formulation to use, but also the choice of amine donor has a decisive impact not only on reaction equilibrium, the inhibition profiles for substrates and products but also on the possibilities for in-situ product removal (ISPR) and technologies for shifting the equilibrium. In a challenging process such as the synthesis of optically pure chiral amines using ω-transaminase, these decisions will have a major influence on the process. Understanding these parameters and their effect on the process for the different reaction systems is important as it will help engineers make the right choices during process design. In this study we have therefore carried out an in depth characterization of different process parameters involved in the production of two chiral amines (S-methylbenzylamine and 3-amino-1-phenylbutane) (Figure 1) to demonstrate the effects of such decisions.

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Publication: Research › Editorial – Annual report year: 2013

**Effect of nitrite, limited reactive settler and plant design configuration on the predicted performance of simultaneous C/N/P removal WWTPs**

This paper describes a modelling study where five new benchmark plant design configurations for biological nutrient removal (A2/O, UCT, JHB, MUCT and BDP-5 stage) are simulated and evaluated under different model assumptions. The ASM2d including electron dependent decay rates is used as the reference model (A1). The second case (A2) adds nitrite as a new state variable, describing nitrification and denitrification as two-step processes. The third set of models (A3 and A4) considers different reactive settlers types (diffusion-limited/non limited). This study analyses the importance of these new model extensions to correctly describe the nitrification behaviour and the carbon source competition between ordinary heterotrophic organisms (OHO) and polyphosphate accumulating organisms (PAO) under certain operation conditions. The economic and environmental aspects when meeting the P discharge limits by adding an external carbon source are also studied.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Universidad Autonoma de Barcelona, Lund University
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The main features of SustainPro are illustrated through a case study of ß-Galactosidase production. The features of the methodology incorporate Life Cycle Assessment analysis and economic analysis. The application and the extended features of SustainPro are evaluated using environmental impact assessment tools and safety indices. The extended SustainPro guides the user through the necessary steps according to the work-flow of the implemented methodology. At the process information/data such as the process flowsheet, the associated mass/energy balance data, and the cost data, extended systematic methodology for sustainable process design (Carvalho et al. 2008 and Carvalho et al. 2009) are described. The generic and flexible nature of the framework (and of the associated data structure) is demonstrated through the formulation and solution of large scale industrial case studies. The case studies are selected from different industrial segments, such as food processing (soybean processing network), water and wastewater management (refinery wastewater treatment and reuse; municipal water treatment) and biorefinery.

**Efficient Information and Data Management in Synthesis and Design of Processing Networks**

Recent developments of Process Systems Engineering (PSE) have focused on different classes of industry-relevant decision-making problems (e.g. planning, scheduling, synthesis and design), under the general framework of Enterprise-Wide Optimization (EWO) (Grossmann, 2005). In EWO, decision-making problems are formulated as superstructure optimization problems, which are solved to identify the optimal decision. In order to formulate large-scale network synthesis problems, large amounts of data are needed to describe: i) the superstructure (in terms of terms of list of alternatives and connections between them); ii) each of the process alternatives (in terms of mass balance, waste emissions, operational, and capital cost); iii) the optimality criterion (in terms of objective function coefficients such as prices), as well as iv) engineering, commercial and regulatory insights and context-related information (such as regulatory limits, and product specs, etc.) (Quaglia et al., 2012). Being those data multisource and multidisciplinary, a consolidation step is required to ensure coherence in problem formulation. The formulation of EWO problems, therefore, requires collecting, consolidating and specifying a large number (typically 1000-100,000) of data (Quaglia et al., submitted). As a result, EWO problem formulation is a time and resource intensive task. Moreover, compilation errors result in faulty problem specifications, and may compromise the quality of the obtained solution. In order to enable industrial use of EWO, therefore, methods and tools for efficient information and data management need to be developed. In this contribution, we present a systematic data architecture, which is integrated in our framework for synthesis and design of processing networks (Quaglia et al., submitted). The data structure is designed to enable automation, systematization and consolidation of the data needed for problem formulation. Those features have been implemented in a software tool for formulation of processing network synthesis and design problems, which guides the user through the steps of problem formulation, integrating automatic data consistency checks and connection to databases of physical properties and process data. Once all data have been specified, the problem is automatically converted into a GAMS readable program, which is executed to solve the optimization problem and identify the optimal processing network, without requiring any further editing from the user. Through the data structure and the formulation software, the workflow for problem formulation is optimized, and time and resources needed to formulate large problems are reduced, while at the same time ensuring internal consistency of the specified data. In this contribution, the framework for synthesis and design of processing network and the data structure are described. The generic and flexible nature of the framework (and of the associated data structure) is demonstrated through the formulation and solution of large scale industrial case studies. The case studies are selected from different industrial segments, such as food processing (soybean processing network), water and wastewater management (refinery wastewater treatment and reuse; municipal water treatment) and biorefinery.

**SustainPro - A tool for systematic process analysis, generation and evaluation of sustainable design alternatives**

Chemical processes are continuously facing challenges from the demands of the global market related to economics, environment and social issues. This paper presents the development of a software tool (SustainPro) and its application to chemical processes operating in batch or continuous modes. The software tool is based on the implementation of an extended systematic methodology for sustainable process design (Carvalho et al. 2008 and Carvalho et al. 2009). Using process information/data such as the process flowsheet, the associated mass/energy balance data and the cost data, SustainPro guides the user through the necessary steps according to work-flow of the implemented methodology. At the end the design alternatives are evaluated using environmental impact assessment tools and safety indices. The extended features of the methodology incorporate Life Cycle Assessment analysis and economic analysis. The application and the main features of SustainPro are illustrated through a case study of ß-Galactosidase production.
Enzymatic production of FAME biodiesel with soluble lipases

Biodiesel is a viable alternative to fossil fuels, and biocatalysis is gaining interest as a greener process. We focus on converting oils to Fatty Acid Methyl Ester (FAME) using soluble lipases, which offer an advantage compared to immobilized enzymes by cost efficiency and ease of implementation. Firstly, we defined the range of interest for process parameters of a low catalyst loading system, intended for single use. Furthermore, we systematically studied the effect and interaction between these parameters. Based on experimental data, a model was developed to evaluate the optimal conditions within the defined operating space concerning: temperature, water content, initial methanol concentration and enzyme content. The identified optimum range was experimentally evaluated, and model findings were confirmed. Another barrier in lipase use in biodiesel production is the higher melting point (m.p.) of certain oils, which is not compatible with the temperature range where lipases are most active. To address this, here we explored a novel production strategy that accommodates the enzymatic requirements with the chemical limits of the substrates. The m.p. of the methyl ester product is lower than that of the starting material. Thus, we have incorporated a varying amount of the product to lower the m.p. of the starting material. Our case study is the reaction of Palm Fatty Acid Distillate (PFAD) to FAME. Conversion rates have been measured with varying temperatures, water concentration, and initial methanol content. The results of this investigation will be presented and discussed in this poster.

Exploring microbial Transglutaminase acceptor substrate specificity: Applications for Biocatalysis

General information
Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, University of Ottawa
Authors: T. Gundersen, M. (Intern), Keillor, J. W. (Ekstern), Pelletier, J. N. (Ekstern)
Publication date: 2013
Event: Poster session presented at 94th Canadian Chemistry Conference & Exhibition, Montreal, Canada.
First principles pharmacokinetic modeling: A quantitative study on Cyclosporin

Unknown dose regimes are typically assessed on animals prior to clinical trials. Recent advances in the evaluation of new leads' efficacy have been achieved by pharmacokinetic modeling. Further improvements, including determination of the drug's mechanism of action and organism biodistribution, require an effective methodology for solving parameter estimation challenges. This article solves the problem of rigorously estimating unknown biochemical reaction and transport parameters from in vivo datasets and identifying whole-body physiologically based pharmacokinetic (PBPK) models. A rat blood circulation model was combined with biotransport, biochemical reactions and metabolism of the immunosuppressant Cyclosporin. We demonstrate the proposed methodology on a case study in Sprague-Dawley rats by bolus iv injections of 1.2, 6 and 30 mg/kg. Key pharmacokinetic parameters were determined, including renal and hepatic clearances, elimination half-life, and mass transfer coefficients, to establish drug biodistribution dynamics in all organs and tissues. This multi-scale model satisfies first principles and conservation of mass, species and momentum. Prediction of organ drug bioaccumulation as a function of cardiac output, physiology, pathology or administration route may be possible with the proposed PBPK framework. Successful application of our model-based drug development method may lead to more efficient preclinical trials, accelerated knowledge gain from animal experiments, and shortened time-to-market of new drugs. © 2013.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, University of Illinois at Chicago
Authors: Mošat', A. (Ekstern), Lueshen, E. (Ekstern), Heitzig, M. (Intern), Hall, C. (Ekstern), Linninger, A. A. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
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Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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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
Fluctuation Solution Theory Properties from Molecular Simulation

The thermodynamic properties obtained in the Fluctuation Solution Theory are based on spatial integrals of molecular TCFs between component pairs in the mixture. Molecular simulation, via either MD or MC calculations, can yield these correlation functions for model inter- and intramolecular potential functions. However, system-size limitations and statistical noise cause uncertainties in the functions at long range, and thus uncertainties or errors in the integrals. A number of methods such as truncation, distance shifting, long-range modeling, transforms, DCF matching, finite-size scaling and adaptive resolution, have been explored to overcome these problems. This chapter reviews the issues and published work associated with using molecular simulation to obtain FST properties. The results suggest that molecular simulation should now be more fully utilized for obtaining quantitative FST thermodynamic properties of solutions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Swedish Defence Research Agency, University of Virginia
Authors: Abildskov, J. (Intern), Wedberg, R. (Ekstern), O’Connell, J. P. (Ekstern)
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Chapter: 6
Main Research Area: Technical/natural sciences
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Framework for assessing stability of biocatalytic oxidations

General information
State: Published
Organisations: Department of Systems Biology, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Ramesh, H. (Intern), Woodley, J. (Intern)
Publication date: 2013
Event: Abstract from BIOTRANS 2013, Manchester, United Kingdom.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Book chapter – Annual report year: 2013

Gas-Solid Heat Exchanger for Cement Production

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, CAPEC-PROCESS, F.L. Smith A/S
Authors: Maarup, C. (Intern), Dam-Johansen, K. (Intern), Clement, K. (Intern), Hjuler, K. (Ekstern)
Number of pages: 312
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Publication information
Publisher: Technical University of Denmark, Department of Chemical and Biochemical Engineering
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Main Research Area: Technical/natural sciences
Electronic versions:
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Source: PublicationPreSubmission
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Publication: Research › Ph.D. thesis – Annual report year: 2014

Generic Modelling Framework for Design and Analysis of Crystallization Operations

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Meisler, K. T. (Intern), Abdul Samad, N. A. F. B. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9429
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Hazard Identification of the Offshore Three-phase Separation Process Based on Multilevel Flow Modeling and HAZOP

HAZOP studies are widely accepted in chemical and petroleum industries as the method for conducting process hazard analysis related to design, maintenance and operation of the systems. Different tools have been developed to automate HAZOP studies. In this paper, a HAZOP reasoning method based on function-oriented modeling, Multilevel Flow Modeling (MFM), is extended with function roles. A graphical MFM editor, which is combined with the reasoning capabilities of the MFM Workbench developed by DTU is applied to automate HAZOP studies. The method is proposed to support the “brain-storming” sessions in traditional HAZOP analysis. As a case study, the extended MFM based HAZOP methodology is applied to an offshore three-phase separation process. The results show that the cause-consequence analysis in MFM can infer the cause and effect of a deviation used in HAZOP and used to fill HAZOP worksheet. This paper is the first paper discussing and demonstrate the potential of the roles concept in MFM to supplement the integrity of HAZOP analysis.

General information
State: Published
Heterologous expression and characterization of bacterial 2-C-methyl-d-erythritol-4-phosphate pathway in Saccharomyces cerevisiae

Transfer of a biosynthetic pathway between evolutionary distant organisms can create a metabolic shunt capable of bypassing the native regulation of the host organism, hereby improving the production of secondary metabolite precursor molecules for important natural products. Here, we report the engineering of Escherichia coli genes encoding the 2-C-methyl-d-erythritol-4-phosphate (MEP) pathway into the genome of Saccharomyces cerevisiae and the characterization of intermediate metabolites synthesized by the MEP pathway in yeast. Our UPLC-MS analysis of the MEP pathway metabolites from engineered yeast showed that the pathway is active until the synthesis of 2-C-methyl-d-erythritol-2,4-cyclodiphosphate, but appears to lack functionality of the last two steps of the MEP pathway, catalyzed by the [4Fe–4S] iron sulfur cluster proteins encoded by ispG and ispH. In order to functionalize the last two steps of the MEP pathway, we co-expressed the genes for the E. coli iron sulfur cluster (ISC) assembly machinery. By deleting ERG13, thereby incapacitating the mevalonate pathway, in conjunction with labeling experiments with U–13C6 glucose and growth experiments, we found that the ISC assembly machinery was unable to functionalize ispG and ispH. However, we have found that leuC and leuD, encoding the heterodimeric iron–sulfur cluster protein, isopropylmalate isomerase, can complement the S. cerevisiae leu1 auxotrophy. To our knowledge, this is the first time a bacterial iron–sulfur cluster protein has been functionally expressed in the cytosol of S. cerevisiae under aerobic conditions and shows that S. cerevisiae has the capability to functionally express at least some bacterial iron–sulfur cluster proteins in its cytosol.
Implementing the next-generation of biocatalytic processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Woodley, J. (Intern)
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Event: Abstract from International Workshop: Advances in Industrial Biotechnology, Sao Carlos, Brazil.
Main Research Area: Technical/natural sciences
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Industry-academia collaboration through the CAPEC industrial consortium

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Authors: Gani, R. (Intern)
Number of pages: 1
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Event: Abstract from Pfizer seminar, Hartford, CT, United States.
Main Research Area: Technical/natural sciences

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Industry-academia collaboration through the CAPEC industrial consortium

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Authors: Gani, R. (Intern)
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Main Research Area: Technical/natural sciences

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Publication: Research › Conference abstract for conference – Annual report year: 2013

In pursuit of benign amide synthesis: novel applications of microbial transglutaminase

General information
State: Published
Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, Universite de Montreal
Authors: T. Gundersen, M. (Intern), Keillor, J. W. (Ekstern), Pelletier, J. N. (Ekstern)
Publication date: 2013
Event: Poster session presented at Gordon Research Conference, Smithfield, RI, United States.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2013

Integrated control of the wastewater system – potentials and barriers
Applying integrated control to a sewer system and wastewater treatment plant often leads to additional benefits for both systems when compared to controlling them independently. However, barriers such as a lack of incentive for utilities to put this type of control in place mean that in practice integrated control of wastewater systems is rarely seen. Ane Loft Mollerup, Morten Grum, Dirk Muschalla, Edwin van Velzen, Peter Vanrolleghem, Peter Steen Mikkelsen and Gurkan Sin outline the benefits of integrated control of wastewater systems.
Introducing uncertainty analysis of nucleation and crystal growth models in Process Analytical Technology (PAT) system design of crystallization processes

This paper presents the application of uncertainty and sensitivity analysis as part of a systematic model-based process monitoring and control (PAT) system design framework for crystallization processes. For the uncertainty analysis, the Monte Carlo procedure is used to propagate input uncertainty, while for sensitivity analysis, global methods including the standardized regression coefficients (SRC) and Morris screening are used to identify the most significant parameters. The potassium dihydrogen phosphate (KDP) crystallization process is used as a case study, both in open-loop and closed-loop operation. In the uncertainty analysis, the impact on the predicted output of uncertain parameters related to the nucleation and the crystal growth model has been investigated for both a one- and two-dimensional crystal size distribution (CSD). The open-loop results show that the input uncertainties lead to significant uncertainties on the CSD, with appearance of a secondary peak due to secondary nucleation for both cases. The sensitivity analysis indicated that the most important parameters affecting the CSDs are nucleation order and growth order constants. In the proposed PAT system design (closed-loop), the target CSD variability was successfully reduced compared to the open-loop case, also when considering uncertainty in nucleation and crystal growth model parameters. The latter forms a strong indication of the robustness of the proposed PAT system design in achieving the target CSD and encourages its transfer to full-scale implementation.
Kinetic model of biodiesel production using immobilized lipase Candida antarctica lipase B

We have designed a kinetic model of biodiesel production using Novozym 435 (Nz435) with immobilized Candida antarctica lipase B (CALB) as a catalyst. The scheme assumed reversibility of all reaction steps and imitated phase effects by introducing various molecular species of water and methanol. The global model was assembled from separate reaction blocks analyzed independently. Computer simulations helped to explore behavior of the reaction system under different conditions. It was found that methanolyis of refined oil by CALB is slow, because triglycerides (T) are the least reactive substrates. Conversion to 95% requires 1.5–6 days of incubation depending on the temperature, enzyme concentration, glycerol inhibition, etc. Other substrates, free fatty acids (F), diglycerides (D) and monoglycerides (M), are utilized much faster (1–2h). This means that waste oil is a better feedstock for CALB. Residual enzymatic activity in biodiesel of standard quality causes increase of D above its specification level because of the reaction 2M↔D+G. Filtration or alkaline treatment of the product prior to storage resolves this problem. The optimal field of Nz435 application appears to be decrease of F, M, D in waste oil before the conventional alkaline conversion. Up to 30-fold reduction of F-content can be achieved in 1–2h, and the residual enzyme (if any) does not survive the following alkaline treatment.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Aarhus University, Novozymes A/S
Authors: Fedosov, S. (Forskerdatabase), Brask, J. (Ekstern), Pedersen, A. K. (Intern), Nordblad, M. (Intern), Woodley, J. (Intern), Xu, X. (Ekstern)
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Scopus rating (2016): CiteScore 2.39 SJR 0.63 SNIP 0.855
Web of Science (2016): Indexed yes
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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
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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
Scopus rating (2009): SJR 0.898 SNIP 1.136
Learning Safety Assessment from Accidents in a University Environment

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Safepark Consultancy
Authors: Jensen, N. (Ekstern), Jørgensen, S. B. (Intern)
Number of pages: 33
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Learning Safety Assessment from Accidents in a University Environment
This contribution describes how a chemical engineering department started learning from accidents during experimental work and ended up implementing an industrially inspired system for risk assessment of new and existing experimental setups as well as a system for assessing potential risk from the chemicals used in the experimental work. These experiences have led to recent developments which focus increasingly on the theoretical basis for modeling and reasoning on safety as well as operational aspects within a common framework. Presently this framework is being extended with barrier concepts both from a practical and a theoretical view.

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Safepark Consultancy
Authors: Jensen, N. (Ekstern), Jørgensen, S. B. (Intern)
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Life cycle assessment in green chemistry: overview of key parameters and methodological concerns

Several articles within the area of green chemistry often promote new techniques or products as 'green' or 'more environmentally benign' than their conventional counterpart although these articles often do not quantitatively assess the environmental performance. In order to do this, life cycle assessment (LCA) is a valuable methodology. However, on the planning stage, a full-scale LCA is considered to be too time consuming and complicated. Two reasons for this have been recognised, the method is too comprehensive and it is hard to find inventory data. In this review, key parameters are presented with the purpose to reduce the time-consuming steps in LCA. In this review, several LCAs of so-called 'green chemicals' are analysed and key parameters and methodological concerns are identified. Further, some conclusions on the environmental performance of chemicals were drawn. For fossil-based platform chemicals several LCAs exists but for chemicals produced with industrial biotechnology or from renewable resources the number of LCAs is limited, with the exception of biofuels, for which a large number of studies are made. In the review, a significant difference in the environmental performance of bulk and fine chemicals was identified. The environmental performance of bulk chemicals are closely connected to the production of the raw material and thereby different land use aspects. Here, a lot can be learnt from biofuel LCAs. In many of the reviewed articles focusing on bulk chemicals a comparison regarding fossil and renewable raw material was done. In most of the comparisons the renewable alternative turned out to be more environmentally preferable, especially for the impact on GWP and energy use. However, some environmental concerns were identified as important to include to assess overall environmental concern, for example eutrophication and the use of land. To assess the environmental performance of green chemicals, quantitative methods are needed. For this purpose, both simple metrics and more comprehensive methods have been developed, one recognised method being LCA. However, this method is often too time consuming to be valuable in the process planning stage. This is partly due to a lack of available inventory data, but also because the method itself is too comprehensive. Here, key parameters for the environmental performance and methodological concerns were described to facilitate a faster and simpler use of LCA of green chemicals in the future.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University
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Web of Science (2015): Indexed yes
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Lipase-catalysed formation of sugar fatty acid ester surfactants using supercritical carbon dioxide as a reaction medium

General information
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Authors: Doherty, C. (Ekstern), Lima Ramos, J. (Intern), Al-Haque, N. (Intern), Turner, N. (Ekstern), Woodley, J. (Intern)
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Managing the Complexity in Chemical Product Engineering

General information
Microbial transglutaminase displays broad acyl-acceptor substrate specificity

The great importance of amide bonds in industrial synthesis has encouraged the search for efficient catalysts of amide bond formation. Microbial transglutaminase (MTG) is heavily utilized in crosslinking proteins in the food and textile industries, where the side chain of a glutamine reacts with the side chain of a lysine, forming a secondary amide bond. Long alkylamines carrying diverse chemical entities can substitute for lysine as acyl-acceptor substrates, to link molecules of interest onto peptides or proteins. Here, we explore short and chemically varied acyl-acceptor substrates, to better understand the nature of nonnatural substrates that are tolerated by MTG, with the aim of diversifying biocatalytic applications of MTG. We show, for the first time, that very short-chain alkyl-based amino acids such as glycine can serve as acceptor substrates. The esterified ω-amino acids Thr, Ser, Cys, and Trp—but not Ile—also showed reactivity. Extending the search to nonnatural compounds, a ring near the amine group—particularly if aromatic—was beneficial for reactivity, although ring substituents reduced reactivity. Overall, amines attached to a less hindered carbon increased reactivity. Importantly, very small amines carrying either the electron-rich azide or the alkyne groups required for click chemistry were highly reactive as acyl-acceptor substrates, providing a robust route to minimally modified, "clickable" peptides. These results demonstrate that MTG is tolerant to a variety of chemically varied natural and nonnatural acyl-acceptor substrates, which broadens the scope for modification of Gln-containing peptides and proteins.
Microreactors and CFD as Tools for Biocatalysis Reactor Design: A case study

Microreactors have been used for acquiring process data while consuming significantly lower amounts of expensive reagents. In this article, the combination of microreactor technology and computational fluid dynamics (CFD) is shown to contribute significantly towards understanding the diffusional properties of the substrate and the product of a biocatalytic reaction. Such knowledge is then applied to design reactor configurations. It has been demonstrated that this kind of knowledge is crucial for the choice and design of reactors. In the discussion, it is highlighted how microreactor-based platforms with similar dimensions to the ones tested here can be used as a screening tool for screening biocatalyst and process alternatives.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Process Engineering and Technology, Technical University of Denmark
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Miniaturized experimental toolbox for \(\omega\)-transaminase technology (BIOINTENSE)

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Pereira Rosinha, I. (Intern), Ringborg, R. H. (Intern), Heintz, S. (Intern), Tufvesson, P. (Intern), Krühne, U. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern)
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Model-based analysis of high shear wet granulation from batch to continuous processes in pharmaceutical production - A critical review
The manufacturing of pharmaceutical dosage forms, which has traditionally been a batch-wise process, is now also transformed into a series of continuous operations. Some operations such as tableting and milling are already performed in continuous mode, while the adaptation towards a complete continuous production line is still hampered by complex steps such as granulation and drying which are considered to be too inflexible to handle potential product change-overs. Granulation is necessary in order to achieve good flowability properties and better control of drug content uniformity. This paper reviews modelling and supporting measurement tools for the high shear wet granulation (HSWG) process, which is an important granulation technique due to the inherent benefits and the suitability of this unit operation for the desired switch to continuous mode. For gaining improved insight into the complete system, particle-level mechanisms are required to be better understood, and linked with an appropriate meso- or macro-scale model. A brief review has been provided to understand the mechanisms of the granulation process at micro- or particle-level such as those involving wetting and nucleation, aggregation, breakage and consolidation. Further, population balance modelling (PBM) and the discrete element method (DEM), which are the current state-of-the-art methods for granulation modelling at micro- to meso-scale, are discussed. The DEM approach has a major role to play in future research as it bridges the gap between micro- and meso-scales. Furthermore, interesting developments in the measurement technologies are discussed with a focus towards inline measurements of the granulation process to obtain experimental data which are required for developing good models. Based on the current state of the developments, the review focuses on the twin-screw granulator as a device for continuous HSWG and attempts to critically evaluate the current process. As a result, a set of open research questions are identified. These questions need to be answered in the future in order to fill the knowledge gap that currently exists both at micro- and macro-scale, and which is currently limiting the further development of the process to its full potential in pharmaceutical applications.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Ghent University
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Model-Based Blend Design: Application to Lubricant Oils

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Model based methods and tools for process systems engineering

Process systems engineering (PSE) provides means to solve a wide range of problems in a systematic and efficient manner. This presentation will give a perspective on model based methods and tools needed to solve a wide range of problems in product-process synthesis-design. These methods and tools need to be integrated with work-flows and data-flows for specific product-process synthesis-design problems within a computer-aided framework. The framework therefore should be able to manage knowledge-data, models and the associated methods and tools needed by specific synthesis-design work-flows and data-flows. In particular, the framework needs to manage models of different types, forms and complexity, together with their associated parameters. The application range of the framework depends very much on the application range of the associated models. Therefore, a modelling tool-box is also a part of the framework. The issue of commercial simulators or software providing the necessary features for product-process synthesis-design as opposed to their development by the academic PSE community will also be discussed. An example of a successful collaboration between academia-industry for the development of model based methods and tools within a computer aided framework for product-process synthesis-design will be highlighted.

General information

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Authors: Gani, R. (Intern)
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Modeling Approaches for Describing Microbial Population Heterogeneity

Although microbial populations are typically described by averaged properties, individual cells present a certain degree of variability. Indeed, initially clonal microbial populations develop into heterogeneous populations, even when growing in a homogeneous environment. A heterogeneous microbial population consists of cells in different states, and it implies a heterogeneous distribution of activities (e.g. respiration, product yield), including different responses to extracellular stimuli. The existence of a heterogeneous cell population may explain the lower productivities obtained for cultivations in large-scale reactors, where substrate and oxygen gradients are observed, in comparison to cultivations in well-mixed bench scale reactors. Population balance models (PBM) have been used in a broad range of applications (e.g. crystallization, granulation, flocculation, polymerization processes) to predict distributions of certain population properties including particle size, mass or volume, and molecular weight. Similarly, PBM allow for a mathematical description of distributed cell properties within microbial populations. Cell total protein content distributions (a measure of cell mass) have been observed to provide a dynamic picture of the interplay between the cells and their surrounding extracellular environment. The work here presented aimed at developing a model framework based on PBM as a tool to further understand the development of heterogeneous microbial populations subjected to varying environmental conditions. Three cases are presented and discussed in this thesis. Common to all is the use of S. cerevisiae as model organism, and the use of cell size and cell cycle position as single-cell descriptors. The first case focuses on the experimental and mathematical description of a yeast population dynamics, in response to the substrate consumption observed during batch cultivation. Cell size and cell cycle position distributions were used to describe the cell population. A two-stage PBM was developed and coupled to an unstructured model describing the extracellular environment. The good agreement between the proposed multi-scale model and experimental data (both the overall physiology and cell size and cell cycle distributions) indicates that a mechanistic model framework is a suitable tool for describing the microbial population dynamics in a bioreactor. The second case provides an extension of the proposed model framework (PBM coupled to an unstructured model) to a continuous cultivation. A compartment model approach was applied for addressing situations where two zones (compartments) are formed due to non-ideal mixing in the bioreactor. In particular, this approach was used in order to assess the impact of the degree of compartmentalization (i.e. deviation from the ideal mixing case) on the population dynamics and overall system performance under various operation conditions (substrate feed concentration and dilution rate). It was possible to conclude that the deviation from ideal mixing may have a significant effect on the observed system dynamics. Moreover, oscillatory pseudo-steady states may be observed for particular combinations of operating conditions and degree of compartmentalization. In the third study attention was paid to the integration of the proposed model framework in a computational (CFD) fluid dynamic model. The anaerobic Growth of a budding yeast population in a continuously run
The microbioreactor was used as an example. The proposed integrated model describes the fluid flow, the local cell size and cell cycle position distributions, as well as the local concentrations of glucose, ethanol and biomass throughout the reactor. This work has proven that the integration of CFD and population balance models, for describing the growth of a microbial population in a spatially heterogeneous reactor, is feasible, and that valuable insight on the interplay between flow and the dynamics of a budding yeast population (e.g. formation of substrate gradients and non-growth zones) is gained. In silico simulation tools, as the one proposed, may be used for hypothesis generation and testing, and when coupled to an experimental set-up may be used for process and reactor design optimization.
Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group- Contribution Method

A group-contribution (GC) property prediction model for estimating the critical micelle concentration (CMC) of nonionic surfactants in water at 25 °C is presented. The model is based on the Marrero and Gani GC method. A systematic analysis of the model performance against experimental data is carried out using data for a wide range of nonionic surfactants covering a wide range of molecular structures. As a result of this procedure, new third order groups based on the characteristic structures of nonionic surfactants are defined and are included in the Marrero and Gani GC model. In this way, those compounds that exhibit larger correlation errors (based only on first- and second-order groups) are assigned to more detailed molecular descriptions, so that better correlations of critical micelle concentrations are obtained. The group parameter estimation has been performed using a data set of 150 experimental measurements covering a large variety of nonionic surfactants including linear, branched, and phenyl alkyl ethoxylates; alkanediols; alkyl mono- and disaccharide ethers and esters; ethoxylated alkyl amines and amides; fluorinated linear ethoxylates and amides; polyglycerol esters; and carbohydrate derivate ethers, esters, and thiols. The model developed consists of linear group contributions, and the critical micelle concentration is estimated using the molecular structure of the nonionic surfactant alone. Compared to other models used for the prediction of the critical micelle concentration, and in particular, the quantitative structure–property relationship models, the developed GC model provides an accurate correlation and allows for an easier and faster application in computer-aided molecular design techniques facilitating chemical process and product design.
Modelling and L1 Adaptive Control of pH in Bioethanol Enzymatic Process

The enzymatic process is a key step in second generation bioethanol production. Pretreated biomass fibers are liquefied with the help of enzymes to facilitate fermentation. Enzymes are very sensitive to pH and temperature and the main control challenge in the nonlinear process is to ensure minimum deviations from the optimal pH level. This article develops a mathematical model for the pH, which has not been reported earlier for this particular process. The new model embeds flow dynamics and pH calculations and serves both for simulation and control design. Two control strategies are then formulated for pH level regulation: one is a classical PI controller; the other an L1 adaptive output feedback controller. Model-based feed-forward terms are added to the controllers to enhance their performances. A new tuning method of the L1 adaptive controller is also proposed. Further, a new performance function is formulated and tailored to this type of processes and is used to monitor the performances of the process in closed loop. The L1 design is found to outperform the PI controller in all tests.

General information
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Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Prunescu, R. M. (Intern), Blanke, M. (Intern), Sin, G. (Intern)
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Modelling and L1 Adaptive Control of Temperature in Biomass Pretreatment

Biomass steam pretreatment is a key process in converting agricultural wastes to bioethanol. The pretreatment occurs in a large pressurized tank called a thermal reactor. Two key parameters influence the successfulness of the process: the reactor temperature, and the retention time. A particle pump pressurizes untreated biomass from atmospheric to reactor pressure with recycled steam from the reactor. This paper formulates a steam mathematical model both for the thermal reactor and the particle pump, which is then used to design an L1 adaptive output feedback controller for the reactor temperature. As steam is recycled from the reactor to pressurize the particle pump, pressure drops and the reactor temperature is disturbed. The main control challenge is to reject these disturbances and keep a steady temperature. The nonlinear process model embeds mass and energy balances, valve characteristics, and enthalpy-pressure and pressure-temperature dependencies. Nonlinear feed-forward terms are added in the control strategy. The process model, the control strategy, the application of the L1 adaptive controller and its tuning method based on minimizing a cost function represent novelties of this paper.

Modelling N₂O dynamics in the engineered N cycle: Observations, assumptions, knowns, and unknowns

Research on nitrous oxide formation in engineered wastewater systems has experienced an exponential development in the recent years due to the important environmental impact of this greenhouse gas. These efforts have crystallized in a large number of publications that aim to identify the importance of the main microbial processes responsible for its production and consumption. The conceptualization of these pathways in mathematical models has the potential to become a key tool to increase our understanding on the complex interrelationships within these ecosystems and develop strategies to minimize the carbon footprint of wastewater treatment plants. Unfortunately, existing model structures are limited to describe the emissions of individual microbial pathways in an attempt to decrease their complexity and facilitate their calibration. The present contribution summarizes the recent developments in this field and makes use of sensitivity analyses, and an in-depth study of model uncertainties to establish experimental protocols that facilitate the calibration and predictive ability of a new generation of more realistic models describing N₂O production during wastewater treatment.
The knowledge of physical and thermodynamic properties of pure components and their mixtures is a basic requirement for performing tasks related to process design, simulation, and optimization and also for performing chemical product design using computer aided molecular/mixture design (CAMD) tools. With an increasing trend in the production rates of edible oils, fats and other lipids, accurate prediction of the necessary properties (pure component and mixture) has become a major concern and issue. The mixtures handled consist of large complex chemicals such as fatty esters, acids, alcohols, glycerides, sterols, etc., with or without the presence of water. Because of the lack of measured data, it is necessary to have available truly predictive but reliable models requiring very little data for their development. A systematic numerical analysis to identify the needs of phase equilibria and related properties in process design and analysis for the production of edible oils and related products has been done and from this analysis the requirements of a database with respect to model development has been established. In total, 333 different phase equilibria systems (91 VLE, 91 LLE, 70 SLE), 80 solubility systems, and around 4500 data points on phase equilibria has been found in addition to 8 pure component properties for 290 lipids. The consistency of the available VLE data has been checked with six tests (Van Ness, Herington or Area, Point or Differential, Infinite Dilution, Pure component and EOS), using a general and robust approach developed by Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST). It was found that most of the data failed, at least one of these tests. Nevertheless, using data-quality factors, all data have been used to regress parameters of UNIFAC model. This procedure has also been repeated for SLE-data, where new thermodynamic consistency tests are proposed. The performance of molecular models (UNIQUAC, UNIFAC, and NRTL) as well as GC+ approach based UNIFAC-CI method is discussed and compared for phase equilibria calculations. For lipids systems, a special set of group-interaction parameters have been determined to make the GC-based models more predictive. These results are then used to obtain interaction parameters for the PC-SAFT to add further predictive power.

Molecular Structure-Based Methods of Property Prediction in Application to Lipids: A Review and Refinement

The paper is a review of the combined group contribution (GC)–atom connectivity index (CI) approach for prediction of physical and thermodynamic properties of organic chemicals and their mixtures with special emphasis on lipids. The combined approach employs carefully selected datasets of different pure component properties to develop simultaneously two parallel models, one based on group contribution and another based on atom connectivity, for each property. The
lipids present in the database are regarded as a separate class, for which special models for pure component properties, primary and temperature dependent, have been developed. For mixtures, properties related to phase equilibria are modeled with GE-based models (UNIQUAC, UNIFAC, NRTL, and combined UNIFAC-CI method). The collected phase equilibrium data for VLE and SLE have been tested for thermodynamic consistency together with a performance evaluation of the GE-models. The paper also reviews the role of the databases and the mathematical and thermodynamic consistency of the measured/estimated data and the predictive nature of the developed models.
Molecular structure based property modeling: Development/Improvement of property models through a systematic property-data-model analysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Hukkerikar, A. S. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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The objective of this work is to develop a method for performing property-data-model analysis so that efficient use of knowledge of properties could be made in the development/improvement of property prediction models. The method includes: (i) analysis of property data and its consistency check; (ii) selection of the most appropriate form of the property model; (iii) selection of the data-set for performing parameter regression and uncertainty analysis; and (iv) analysis of model prediction errors to take necessary corrective steps to improve the accuracy and the reliability of property models.

To make the property-data-model analysis fast and efficient, an approach based on the "molecular structure similarity criteria" to identify molecules (mono-functional, bi-functional, etc.) containing specified set of structural parameters (that is, groups) is employed. The method has been applied to a wide range of properties of pure compounds. In this work, however, the application of the method is illustrated for the property modeling of normal melting point, enthalpy of fusion, enthalpy of formation, and critical temperature. For all the properties listed above, it has been possible to achieve significant improvements in the performance of their models. The improved model for enthalpy of formation yields an average absolute deviation of 1.75 kJ/mol which is well within the required chemical accuracy. All of the available experimental data-points are used for the regression purpose. However, a method for selecting a minimum data-set for the parameter regression is also discussed for the cases where it is preferred to retain some data-points from the total data-set to test the reliability of predictions for validation purposes.
Molecular Thermodynamic Modeling of Fluctuation Solution Theory Properties

Fluctuation Solution Theory provides relationships between integrals of the molecular pair total and direct correlation functions and the pressure derivative of solution density, partial molar volumes, and composition derivatives of activity coefficients. For dense fluids, the integrals follow a relatively simple corresponding-states behavior even for complex systems, show welldefined relationships for infinite dilution properties in complex and near-critical systems, allow estimation of mixed-solvent solubilities of gases and pharmaceuticals, and can be expressed by simple perturbation models for densities and gas solubilities, including ionic liquids and complex mixtures such as coal liquids. The approach is especially useful in systems with strong nonidealities. This chapter describes successful application of such modeling to a wide variety of systems treated over several decades and suggests how to test Equation of State mixing rules.

Optimal Design of Microalgal Biomass Processing Network

In this study, we propose a mixed integer nonlinear programming (MINLP) model for superstructure based optimization of biodiesel production from microalgal biomass. The proposed superstructure includes a number of major processing steps for the production of biodiesel from microalgal biomass, such as the harvesting of microalgal biomass, pretreatments including drying and cell disruption of harvested biomass, lipid extraction, transesterification, and post-transesterification purification. The proposed model is used to find the optimal processing pathway among the large number of potential pathways that exist for the production of biodiesel from microalgae. The proposed methodology is tested by implementing on a specific case with different choices of objective functions. The MINLP model is implemented and solved in GAMS using a database built in Excel. The results from the optimization are analyzed and their significances are discussed.
Many traditional bio-processes are operated in semi-batch mode, in which, a feed stream containing substrate and or nutrients is fed into the reactor during the course of the reaction. One key advantage of a semi-batch operation is that regulation of the substrate concentration has been found to be effective in mitigating the effects of substrate inhibition. Using enzymatic biodiesel production as a case study, the volumetric productivity of the reactor is increased while minimizing inactivation of the enzyme due to the alcohol. This is done by using a simple optimization routine where the substrate (both the vegetable oil and alcohol) feed rate/concentration is manipulated simultaneously. The results of the simulation were tested in the laboratory and are sufficiently positive to suggest the implementation of a feeding strategy for large scale enzymatic biodiesel production.

Optimization of Substrate Feeding for Enzymatic Biodiesel Production

Many traditional bio-processes are operated in semi-batch mode, in which, a feed stream containing substrate and or nutrients is fed into the reactor during the course of the reaction. One key advantage of a semi-batch operation is that regulation of the substrate concentration has been found to be effective in mitigating the effects of substrate inhibition. Using enzymatic biodiesel production as a case study, the volumetric productivity of the reactor is increased while minimizing inactivation of the enzyme due to the alcohol. This is done by using a simple optimization routine where the substrate (both the vegetable oil and alcohol) feed rate/concentration is manipulated simultaneously. The results of the simulation were tested in the laboratory and are sufficiently positive to suggest the implementation of a feeding strategy for large scale enzymatic biodiesel production.
substrate (both the vegetable oil and alcohol) feed rate/concentration is manipulated simultaneously. The results of the simulation were tested in the laboratory and are sufficiently positive to suggest the implementation of a feeding strategy for large scale enzymatic biodiesel production.
**pH variation and influence in an autotrophic nitrogen removing biofilm system using an efficient numerical solution strategy**

A pH simulator consisting of an efficient numerical solver of a system of nine nonlinear equations was constructed and implemented in the modeling software MATLAB. The pH simulator was integrated in a granular biofilm model and used to simulate the pH profiles within granules performing the nitrification-anammox process for a range of operating points. The simulation results showed that pH profiles were consistently increasing with increasing depth into the granule, since the proton producing aerobic ammonium oxidizers (AOB) were located close to the granule surface. Despite this pH profile, more NH₃ was available for AOB than for anaerobic ammonium oxidizers (AnAOB), located in the center of the granules. However, operating at a higher oxygen loading resulted in steeper changes in pH over the depth of the granule and caused the NH₃ concentration profile to increase from the granule surface towards the center. The initial value of the background charge and influent bicarbonate concentration were found to greatly influence the simulation result and should be accurately measured. Since the change in pH over the depth of the biofilm was relatively small, the activity potential of the microbial groups affected by the pH did not change more than 5% over the depth of the granules.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
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Scopus rating (2015): SJR 0.466 SNIP 0.599 CiteScore 1.19
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
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Practical Implementations of Advanced Process Control for Linear Systems

This paper describes some practical problems encountered, when implementing Advanced Process Control, APC, schemes on linear processes. The implemented APC controllers discussed will be LQR, Riccati MPC and Condensed MPC controllers illustrated by simulation of the Four Tank Process and a linearised CSTR. Advantages and disadvantages of these controllers will be discussed. All three controller types shows a set of common undesirable characteristics, which must be accounted for. At the end of the evaluation horizon the "optimal" solution has an unstable characteristics, which can be suppressed be selecting dierent control and evaluation horizon. Depending of the degrees of freedom, oset-free control of a number of the controlled variables can be achieved by integration of the innovation errors and introduction of noise models. If the measured or unmeasured disturbances increases, oset-free control cannot be achieved without violation of process constraints. A target calculation function can be used to calculate the optimal achievable target for the process. The use of hard and soft constraints for process input constraints in the MPC controllers, ensures feasible solutions. The computational load as function of controllers type, Model dimension and constraint type will be discussed. Finally the special requirements set by processes including a pure integration dynamics will be illustrated by a linearised CSTR process. The simulated results presented, will later on be implemented on and demonstrated on pilot plant equipment on the department of Chemical Engineering DTU Lyngby.

General information
State: Published
**Practical Implementations of Advanced Process Control for Linear Systems**

Most advanced process control systems are based on Model Predictive Control (MPC). In this paper we discuss three critical issues for the practical implementation of linear MPC for process control applications. The first issue is related to offset free control and disturbance models; the second issue is related to the use of soft output constraints in MPC; and the third issue is related to the computationally efficient solution of the quadratic program in the dynamic regulator of the MPC.

We have implemented MPC in .Net using C# and the MPCMath library. The implemented MPC is based on the target-regulator structure. It enables offset free control; it can be computed efficiently on-line using several optimization algorithms; and accommodates soft constraint for the outputs and for shaping the set-point tracking penalty function. We report selected observations using this implementation and discuss their practical implications for process control. If the control and evaluation intervals are chosen too short, the predicted behaviour of the controllers may have unstable characteristics. Depending of the degrees of freedom, offset-free control of a number of the controlled variables can be achieved by introduction of noise models and integration of the innovation errors. If the disturbances increases, offset-free control cannot be achieved without violation of process constraints. A target calculation function is used to calculate the optimal achievable target for the process. The use of soft constraints for process output constraints in the MPC controllers, ensures feasible solutions. The computational load as function of controllers type, model dimension and constraint type are shown.

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**Predicting Surfactant-related Properties for Chemical-based Product Design**

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**General information**

**State:** Published

**Organisations:** Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering

**Authors:** Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)

**Number of pages:** 1

**Publication date:** 2013

**Event:** Abstract from 2013 AIChE Annual Meeting, San Francisco, CA, United States.

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

**Bibliographical note**

**Oral presentation**

**Source:** dtu

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**Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2013
Prediction of thermo-physical properties of liquid formulated products

The objective of this chapter is to give an overview of the models, methods and tools that may be used for the estimation of liquid formulated products. First a classification of the products is given and the thermo-physical properties needed to represent their functions are listed. For each property, a collection of the available models are presented according to the property type and the model type. It should be noted, however, that the property models considered or highlighted in this chapter are only examples and are not necessarily the best and most accurate for the corresponding property.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Conte, E. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 36
Publication date: 2013

Prediction of vapor pressure and heats of vaporization of edible oil/fat compounds by group contribution

In the present work, a group contribution method is proposed for the estimation of vapor pressures and heats of vaporization of organic liquids found in edible fat/oil and biofuel industries as a function of temperature. The regression of group contribution parameters was based on an extensive databank (2036 values) composed by fatty compounds, i.e., fatty acids, methyl-, ethyl-, propyl- and butyl- esters, fatty alcohols, tri-, di- and monoacylglycerols and hydrocarbons. This new methodology gives improved predictions when compared to a prior group contribution equation (Ceriani and Meirelles, 2004) due to the inclusion of new experimental data for fatty esters and partial acylglycerols (besides hydrocarbons) and critical points, and a new temperature dependency. Heats of vaporization are properly described as a function of reduced temperature up to the critical condition.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Universidade Estadual de Campinas, Virginia Polytechnic Institute and State University
Authors: Ceriani, R. (Ekstern), Gani, R. (Intern), Liu, Y. (Ekstern)
Pages: 53-59
Publication date: 2013
Main Research Area: Technical/natural sciences

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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
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Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
The implementation of new biocatalytic processes can be a very challenging procedure, which can require several stages of screening, characterization and evaluation prior to scale-up. Indeed, several process parameters, with different weights on the final process costs, need to be considered side-by-side. Process design and economic evaluation represent a very important part of the early process development stage. However, often the parameters set at these initial stages are based on assumptions. Therefore, a laboratory scale characterization of the biocatalyst and different process options are important in order to eliminate infeasible routes. This work illustrates the Laboratory scale characterization of different process options for the asymmetric synthesis of chiral amines catalysed by \( \omega \)-transaminase (\( \omega \)-TAm). The studied process options include: (i) the immobilization of the biocatalyst to improve its stability and allow recycling and easy separation; (ii) the use of controlled release of substrate...
(fed-batch) or in situ substrate supply – (ISSS) to decrease substrate inhibition and deal with the substrate low solubility; and (iii) the use of in situ product (ISPR) and co-product removal (IScPR) to respectively alleviate product inhibition and shift the reaction equilibrium. From an academic point of view, more important than the implementation of these technologies to a specific example, is the development of a general methodology that can be later applied in other cases. Hence, this work has also focused on development of comprehensive screening methodologies and guidelines to aid (i) the selection and characterization of suitable biocatalysts for the process; (ii) the selection and characterization of suitable carriers for immobilization of (S)- and (R)-selective ω-TAm; and (iii) the selection of suitable polymeric resins for product removal. The work has been performed in collaboration with c-LEcta GmbH (Leipzig, Germany) and DSM Innovative Synthesis (Geleen, The Netherlands) who supplied the enzymes for the case study, making possible the successful demonstration of the screening methodologies developed. Furthermore, the work addresses several practical questions regarding to the implementation of the process strategies mentioned above.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Lima Afonso Neto, W. (Intern), Woodley, J. (Intern), Tufvesson, P. (Intern)
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Main Research Area: Technical/natural sciences
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Publication: Research › Ph.D. thesis – Annual report year: 2013

Process intensification for bioprocesses

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Woodley, J. (Intern)
Publication date: 2013
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Main Research Area: Technical/natural sciences
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Process strategies for implementing ω-transaminase catalysed reactions

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Lima Afonso Neto, W. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Process strategies for implementing ω-transaminase catalysed reactions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Lima Afonso Neto, W. (Intern), Schwarze, D. (Ekstern), Vogel, A. (Ekstern), Panella, L. (Ekstern), Schurmann, M. (Ekstern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Publication date: 2013
Event: Abstract from BIOTRANS 2013, Manchester, United Kingdom.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013
Process Technology for Immobilized Lipase-catalyzed Process Technology for Immobilized Lipase-catalyzed

Biocatalysis has attracted significant attention recently, mainly due to its high selectivity and potential benefits for sustainability. Applications can be found in biorefineries, turning biomass into energy and chemicals, and also for products in the food and pharmaceutical industries. However, most applications remain in the production of high-value fine chemicals, primarily because of the expense of introducing new technology. In particular lipase-catalyzed synthesis has already achieved efficient operations for high-value products and more interesting now is to establish opportunities for low-value products. In order to guide the industrial implementation of immobilized-lipase catalyzed reactions, especially for high-volume low-value products, a methodological framework for dealing with the technical and scientific challenges and establishing an efficient process via targeted scale-down experimental work is described in this thesis. The methodology uses economic targets to test options characterized via a set of tools. In order to validate the methodology, two processes based on immobilized lipase-catalysis have been studied: transesterification and esterification of vegetable oils for the production of biodiesel. The two processes are focused on the conversion of the two main components of vegetable oil materials, glyceride esters and free fatty acids respectively, into fatty acid alkyl esters. Although biodiesel is conventionally prepared via chemical-catalyzed transesterification of vegetable oils with methanol to produce fatty acid methyl esters (FAME), this work has been focused on the production of fatty acid ethyl esters (FAEE) with bioethanol due to the expected improved sustainability of this type of biodiesel. A key reaction characteristic of the immobilized lipase-catalyzed transesterification is that it is multi-phasic system. The by-product glycerol can potentially impose inhibitory effects on immobilized lipases and likewise the un-dissolved ethanol can inhibit the lipase. The options for addressing these issues can be used as the basis for selecting the biocatalyst and the reactor (e.g. a hydrophobic carrier for the immobilized lipase and the capabilities to provide sufficient mixing as well as stepwise/continuous feeding of ethanol to the reactor). An STR is efficient for batch operation while a PBR is efficient for a continuous production. An STR can more easily provide sufficient external mass transfer for a reaction, but will lead to more mechanical damage of the biocatalyst particles, than a PBR. A reactor combination of CSTR with PBR can couple the advantages of both, delivering an efficient continuous process. The second case study (esterification) shares some similar process characteristics to the first case (e.g. the multi-phasic nature). However, instead of glycerol, water shows a great impact on the extent of reaction. The removal of water should therefore be feasible during the operation of the reactor, either intermittently or preferably in situ. Highly anhydrous reaction conditions and the smaller substrates for this reaction place particular requirements on the lipase. In order to validate the established processes at a larger scale, both lipase-catalyzed transesterification and esterification developed in the lab-scale STRs have been carried out in pilot-scale STRs. Results in both scale STRs correlate well with respect to the biocatalyst performance and mechanical stability. Once the technical and scientific challenges of the process have been addressed, it is of course important to evaluate its economic and environmental feasibility. To that end, process evaluation has been performed for six processes composed of transesterification and product purification for making 'in-
spec’ biodiesel and the conventional chemical process is taken as a benchmark for comparison. The optimal process is a process composed of lipase-catalyzed transesterification with ‘in-spec’ biodiesel product as output with less feedstock input and waste production and much saved energy from the absence of product purification.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Xu, Y. (Intern), Woodley, J. (Intern), Nordblad, M. (Intern)
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Publication: Research › Ph.D. thesis – Annual report year: 2012

**Production of Phenol from Cumene - Systematic and Efficient Design Method**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Denmark
Authors: Bertran, M. (Intern), Galvanin, S. (Ekstern), Mattei, M. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_Production_of_.pdf
Source: PublicationPreSubmission
Source-ID: 102281303
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

**Protein engineering of enzymes for process applications**
Scientific progress in the field of enzyme modification today enables the opportunity to tune a given biocatalyst for a specific industrial application. Much work has been focused on extending the substrate repertoire and altering selectivity. Nevertheless, it is clear that many new forthcoming opportunities will be targeted on modification to enable process application. This article discusses the challenges involved in enzyme modification focused on process requirements, such as the need to fulfill reaction thermodynamics, specific activity under the required conditions, kinetics at required concentrations, and stability. Finally, future research directions are discussed, including the integration of biocatalysis with neighboring chemical steps.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Woodley, J. M. (Intern)
Pages: 310-316
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Web of Science (2017): Indexed Yes
PSE For Solvent Applications: A Generic Computer-aided Solvent Selection and Design Framework

Solvents are widely used across a number of industries in many applications such as separation agents, reaction mediums, cleaning agents and product carriers. Selection of optimal solvents in these applications is mostly based on previous experiences and experimental trial and error. A process system engineering view that emphasizes a systematic and generic solution framework to solvent selection problems is presented. The framework integrates different methods and tools to manage the complexity and solve a wide range of problems in efficient and flexible manner. Its software implementation, SolventPro, features a set of problem specific templates for various solvent related problems such as, solvents for organic synthesis, solvent-based separations (vapour-liquid, liquid-liquid, solid-liquid equilibrium systems), solvents for phase transfer catalysis reactions, solvents for pharmaceutical industry (API solubility), solvents in formulations and as cleaning agents. The template is expected to guide the average user through the essential and desirable steps in solvent selection and design. The expert may also use the general interface and create their own template for the types of solvent related problems they usually solve. The solvents database currently contains information about more than 1000 organic solvents and their properties -including environmental and transportation - and about 1000 ionic liquids useful for extraction-based separation processes. Property models library include group contribution plus models for pure component and mixture property predictions that allow the selection and design of innovative solvent based processes and products. The application of the framework is highlighted with a number of solvent selection problems from industry.
Purification of 5-hydroxymethylfurfural (hmf) by crystallization
This invention relates to an efficient procedure for purifying HMF by crystallization at low temperature from an organic solvent.

Reaction Engineering of Biocatalytic Enantioselective Reduction: A Case Study for Aliphatic Ketones
Previously, it could be demonstrated, that the monophasic, enzymatic reduction of aliphatic 2-ketones into the corresponding (R)-2-alcohols is an adequate and viable method as carried out in a cascade of two enzyme–membrane reactors (Leuchs, S.; Na’amnieh, S. N.; Greiner, L. Green Chemistry 2013, 15, 167–176.). In the present work, the process metrics of the ketone reduction were calculated. A cost analysis revealed that the enzyme costs are negligible, but the cost for nicotinamide cofactor NADP+ is dominating the overall cost of the chemical raw material followed by the ionic liquid (TEGO IL K5) used as solubiliser and the buffer. The overall cost of chemicals was €148/kg product. To assess the environmental impact of the process, the E-factor (kg waste/kg product) 132 and the process mass intensity (PMI, kg substrate/kg product) were calculated. A process model based on initial rate experiments was elaborated and used to improve the process under cost and environmental aspects. Applying several measures to enhance the cofactor utilisation, the cost base could be reduced by 65% and the E-factor (PMI) to 17 (18).
Reactor selection for multi-step enzymatic reactions

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Reduction of a single granule drying model: An essential step in preparation of a population balance model with a continuous growth term

The development of a Population Balance Model (PBM) for a pharmaceutical granule drying process requires a continuous growth term; the latter actually represents the drying process as the moisture content is the internal coordinate of the PBM. To establish such a PBM, a complex drying model for a single granule needs reduction in complexity. The starting point is a detailed model that describes the drying behavior of single pharmaceutical granules. A Global Sensitivity Analysis (GSA) was performed to detect the most sensitive degrees of freedom in the model as these need to be retained in the reduced model. Simulations of the complex drying model were, in a next phase, used to develop the reduced model, which describes the decrease of the moisture content in function of the gas temperature. The developed reduced model was then included in a Population Balance Equation (PBE) to describe the drying behavior of a population of granules. © 2012 American Institute of Chemical Engineers AIChE J, 59: 1127–1138, 2013
Rengøring på slagterier og mejerier i Danmark: Udvikling af fremtidens effektive, ressourcebesparende teknologier

General information
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Organisations: Office for Innovation & Sector Services, Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Micro- and Nanotechnology
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Publication: Research › Report – Annual report year: 2013
Scale-up and intensification of (S)-1-(2-chlorophenyl)ethanol bioproduction: Economic evaluation of whole cell-catalyzed reduction of o-Chloroacetophenone

Escherichia coli cells co-expressing genes coding for Candida tenuis xylose reductase and Candida boidinii formate dehydrogenase were used for the bioreduction of o-chloroacetophenone with in situ coenzyme recycling. The product, (S)-1-(2-chlorophenyl)ethanol, is a key chiral intermediate in the synthesis of polo-like kinase 1 inhibitors, a new class of chemotherapeutic drugs. Production of the alcohol in multi-gram scale requires intensification and scale-up of the biocatalyst production, biotransformation, and downstream processing. Cell cultivation in a 6.9-L bioreactor led to a more than tenfold increase in cell concentration compared to shaken flask cultivation. The resultant cells were used in conversions of 300 mM substrate to (S)-1-(2-chlorophenyl)ethanol (e.e. >99.9%) in high yield (96%). Results obtained in a reaction volume of 500 mL were identical to biotransformations carried out in 1 mL (analytical) and 15 mL (preparative) scale. Optimization of product isolation based on hexane extraction yielded 86% isolated product. Biotransformation and extraction were accomplished in a stirred tank reactor equipped with pH and temperature control. The developed process lowered production costs by 80% and enabled (S)-1-(2-chlorophenyl)ethanol production within previously defined economic boundaries. A simple and efficient way to synthesize (S)-1-(2-chlorophenyl)ethanol in an isolated amount of 20 g product per reaction batch was demonstrated. Biotechnol. Bioeng. 2013; 110: 2311–2315. © 2013 Wiley Periodicals, Inc.
Selection and design of solvents

Solvents are liquid solutions consisting of one or more chemicals. They have a very wide use and their use is not necessarily restricted to the process industries. This lecture will discuss the different roles and uses of solvents in chemical products and processes that manufacture them. With increasing interest on issues such as waste, sustainability, environmental impact and green chemistry, the selection and design of solvents have become important problems that need to be addressed during chemical product-process design and development. Systematic methods and tools suitable for selection and design of solvents will be presented together with application examples. The selection problem is defined as finding known chemicals that match the desired functions of a solvent for a specified set of applications. The design problem is defined as finding the molecular structure (or mixture of molecules) that match the desired functions of a solvent for a specified set of applications. Use of organic chemicals and ionic liquids as solvents will be covered.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from 23rd Croatian Meeting of Chemists and Chemical Engineers, Osijek, Croatia.
Main Research Area: Technical/natural sciences

Relations
Activities:
Selection and design of solvents
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013
Selection of controlled variables in bioprocesses. Application to a SHARON-Anamox process for autotrophic nitrogen removal

Selecting the right controlled variables in a bioprocess is challenging since the objectives of the process (yields, product or substrate concentration) are difficult to relate with a given actuator. We apply here process control tools that can be used to assist in the selection of controlled variables to the case of the SHARON-Anamox process for autotrophic nitrogen removal.

Self-optimising control of sewer systems

The design of sewer system control is a complex task given the large size of the sewer networks, the transient dynamics of the water flows and the stochastic nature of rainfall. This contribution presents a generic methodology for the design of a self-optimising controller in sewer systems. The definition of an optimal performance was carried out by through 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.

Self-optimising control of sewer systems

Self-optimising control is a useful concept to select optimal controlled variables from a set of candidate measurements in a systematic manner. In this study, use self-optimizing control tools and apply them to the specific features of sewer systems, e.g. the continuously transient dynamics, the availability of a large number of measurements, the stochastic and unforeseeable character of the disturbances (rainfall). Using a subcatchment area in the Copenhagen sewer system as a case study we demonstrate, step by step, the formulation of the self-optimising control problem. The final result is an improved control structure aimed at optimizing the losses for a given control objective, here the minimization of the combined sewer overflows despite rainfall variations.
Simulation study of microbioreactor configurations for production of optically pure chiral amines

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Pereira Rosinha, I. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Krühne, U. (Intern)
Publication date: 2013
Event: Abstract from International Conference on Implementation of Microreactor Technology into Biotechnology (IMTB2013), Cavtat, Croatia.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Software Integration of Life Cycle Assessment and Economic Analysis for Process Evaluation

This study is focused on the sustainable process design of bioethanol production from cassava rhizome. The study includes: process simulation, sustainability analysis, economic evaluation and life cycle assessment (LCA). A steady state process simulation if performed to generate a base case design of the bioethanol conversion process using cassava rhizome as a feedstock. The sustainability analysis is performed to analyze the relevant indicators in sustainability metrics, to definedesign/retrofit targets for process improvements. Economic analysis is performed to evaluate the profitability of the process. Also, simultaneously with sustainability analysis, the life cycle impact on environment associated with bioethanol production is performed. Finally, candidate alternative designs are generated and compared with the base case design in terms of LCA, economics, waste, energy usage and environmental impact in order to identify the most sustainable design for the production of ethanol. The capacity for ethanol production from cassava rhizome is set to 150,000 liters/day, which is about 1.3 % of the total demand of ethanol in Thailand. LCA on the base case design pointed to large amounts of CO2 and CO emissions (related to combustion engine from transportation), biowaste and waste water that are released from the distillation columns, which affect the terrestrial ecotoxicity. Sustainability analysis on the base case pointed to a large waste of the water and lignin, which were then targeted for potential improvement.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Chulalongkorn University
Authors: Kalakula, S. (Ekstern), Malakula, P. (Ekstern), Siemanonda, K. (Ekstern), Gani, R. (Intern)
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Special issue - The 60th Anniversary of the European Federation of Chemical Engineering (EFCE)

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Pages: 1791-1792
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Study of Crystallization Kinetics Within a Generic Modelling Framework

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Loughborough University
Publication date: 2013
Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Superstructure development and optimization for design/retrofit of municipal wastewater treatment plants

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Bozkurt, H. (Intern), Quaglia, A. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Publication date: 2013
Event:
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9027
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Superstructure optimization of biodiesel production from microalgal biomass

In this study, we propose a mixed integer nonlinear programming (MINLP) model for superstructure based optimization of biodiesel production from microalgal biomass. The proposed superstructure includes a number of major processing steps for the production of biodiesel from microalgal biomass, such as harvesting of microalgal biomass, pretreatments including drying and cell disruption of harvested biomass, lipid extraction, transesterification, and post-transesterfication purification. The proposed model is used to find the optimal processing pathway among the large number of potential pathways that exist for the production of biodiesel from microalgae. The proposed methodology is tested by implementing on a specific case study. The MINLP model is implemented and solved in GAMS using a database built in Excel. The results from the optimization are analyzed and their significances are discussed.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Korea Advanced Institute of Science & Technology
Authors: Rizwan, M. (Ekstern), Lee, J. H. (Ekstern), Gani, R. (Intern)
Pages: 111-116
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Publisher: Elsevier Science
ISBN (Print): 9781629937267
Main Research Area: Technical/natural sciences
Biodiesel, Microalgae, Superstructure optimization, Mixed integer nonlinear programming, Biorefinery
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013
Sustainable and Intensified Design of a Biodiesel Production Process

The growing concerns about the global warming and greenhouse gas emissions (GHG) have led to an increase in the interest to produce fuel from biomass and from the fact that such fuels can relieve the reliance on imported oil and price. To this end, numerous production facilities are being set up, at different scales and using different methods of manufacture based on different raw materials and component properties [1]. It is therefore timely to study the sustainability and feasibility of these various manufacturing routes. Therefore, finding the best alternative and design with minimum environmental impact and maximum profitability is needed. In this work a computer-aided framework for process synthesis and process intensification is applied for sustainable production of biodiesel from pure/waste palm oil as the feedstock. This approach examines several biodiesel processing routes that were collected through available data and current technologies reported in the literature. Using this information, a generic superstructure of processing routes was created that described a network of configurations representing multiple designs for the production of biodiesel. Therefore, based on the currently known technologies, this superstructure includes all possible alternatives. The next step was to analyze the superstructure in terms of economic and sustainability metrics. This was done by first performing simulation to obtain the steady state mass and energy balance data for the entire superstructure. These data were then used for a sustainability analysis [2] where a set of calculated closed- and open-path indicators were employed to identify the structural bottlenecks within the superstructure. Based on this analysis the number of process alternatives within the superstructure was reduced and a set of feasible flowsheet alternatives were identified. These were further reduced through economic and lifecycle assessment analysis (LCA) to determine the alternative that best matched a specified set of performance criteria (or design targets). A rigorous simulation was performed on this flowsheet, which at this stage was considered as the base case design for the next step of the framework. To further improve the base case design, process intensification was considered [3] with the targets set by LCA, economic and sustainability analyses in the previous step. Out of the three available levels for achieving PI, the phenomena-level, which is the lowest level of aggregation, was considered so that potentially new and improved alternatives to the base case design could be obtained. The objective (or target) for the intensified process design was to overcome the bottlenecks of the base case design. The optimization problem was further refined in terms of logical, operational, structural constraints, using a PI knowledge base tool. The next step was to identify the phenomena representing the tasks performed within the base case design and the operating window of each phenomenon, by applying thermodynamic insights [4] and the PI knowledge base. Next, the phenomena needed to overcome all identified process bottlenecks were identified, sorted in terms of operation (task) types and the phenomena present in them, and, screened using structural, operational and thermodynamic information. Note that different combinations of phenomena can perform the same specified task. The phenomena were then combined according to a set of rules to form unit operations, which in turn were combined to form new and innovative process alternatives. Finally, from the remaining set of feasible intensified process alternatives, the best in terms of economic and environmental sustainability was identified. For the case of biodiesel production, the intensified process alternative turned out to be the most economical and more sustainable than other alternatives. The computer-aided methods and tools used in this work are: SustainPro (method and tool for process sustainability analysis), ECON (method and tool for process economic analysis), LCSoft (method and tool for process lifecycle assessment analysis) and process simulation software (e.g. PRO/II, ASPEN Plus, ICAS). They are all used in an integrated framework for process synthesis.
Sustainable Intensified Process Retrofit for the Production of MDI

Process intensification (PI) is a means by which processes can be made more efficient and sustainable at different levels, the unit operations, functional and phenomena levels. Therefore PI can be used for making process improvements at the functional level for the production of an important polyurethane, methylene diphenyl-di-isocyanate (MDI).

General information
State: Published
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Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::8408
Publication: Research - peer-review › Poster – Annual report year: 2013

Sustainable Process Design of Biofuels: Bioethanol Production from Cassava rhizome

This study is focused on the sustainable process design of bioethanol production from cassava rhizome. The study includes: process simulation, sustainability analysis, economic evaluation and life cycle assessment (LCA). A steady state process simulation is performed to generate a base case design of the bioethanol conversion process using cassava rhizome as a feedstock. The sustainability analysis is performed to analyze the relevant indicators in sustainability metrics, to defined design/retrofit targets for process improvements. Economic analysis is performed to evaluate the profitability of the process. Also, simultaneously with sustainability analysis, the life cycle impact on environment associated with bioethanol production is performed. Finally, candidate alternative designs are generated and compared with the base case design in terms of LCA, economics, waste, energy usage and environmental impact in order to identify the most sustainable design for the production of ethanol. The capacity for ethanol production from cassava rhizome is set to 150,000 liters/day, which is about 1.3% of the total demand of ethanol in Thailand. LCA on the base case design pointed to large amounts of CO2 and CO emissions (related to combustion engine from transportation), biowaste and waste water that are released from the distillation columns, which affect the terrestrial ecotoxicity. Sustainability analysis on the base case pointed to a large waste of the water and lignin, which were then targeted for potential improvement.

General information
State: Published
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Sustainable Process Design of Lignocellulose based Biofuel

Worldwide energy demand has increased steadily as the world population has grown and more countries have become industrialized. The major energy sources of the world still depend on fossil fuels, which are also the main sources for carbon dioxide emission. As the fossil fuels always pass through a combustion processing step, carbon dioxide and other important greenhouse gases are released. This is considered non-renewable and non-sustainable energy and may be one
of the major causes of global warming and therefore, climate change concerns coupled with high oil prices. This is driving efforts to increase the production and use of alternative and sustainable energy sources as rapidly as possible. Biofuel is a type of alternative energy that can be produced from many sources including sugar substances (such as sugarcane juice and molasses), starchy materials (such as corn and cassava), and lignocellulosic materials such as agricultural residual, straw and wood chips, the residual from wood industry. However, those sugar and starchy materials can be used not only to make biofuels but they are also food sources. Thus, lignocellulosic materials are interesting feed-stocks as they are inexpensive, abundantly available, and are also non-food crops. In this respect, Cassava rhizome has several characteristics that make it a potential feedstock for fuel ethanol production. It has high content of cellulose and hemicelluloses.

The objective of this paper is to present a study focused on the sustainable process design of bioethanol production from cassava rhizome using various computer aided tools through a systematic and efficient work-flow. The study includes process simulation, sustainability analysis, economic evaluation and life cycle assessment (LCA) according to a well-defined workflow that guarantees the determination of sustainable process options, if they exist. The paper will highlight an improved alternative process design compared to a base case (published) design in terms of production cost, waste, energy usage and environmental impacts, criteria that are associated with sustainable process design. The final process design includes 39 unit operations, has a capacity of 150,000 L/day and produces dry ethanol (approximately 13.0% of cassava rhizome is converted to ethanol).

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Number of pages: 1
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Sustainable, Process design, Bioethanol, Lignocellulosic materials, Life cycle assessment

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Synthesis and Design of Biorefinery Processing Networks with Uncertainty and Sustainability analysis
Chemical industries usually rely on fossil based feedstock, which is a limited resource. In view of increasing energy demands and the negative environmental and climate effects related to the use of fossil based fuels, this motivates the development of new and more sustainable technologies for processing renewable feedstocks, with the aim of bridging the gap for fuel, chemical and material production. This project is focusing on biorefinery network design, in particular for early stage design and development studies. Optimal biorefinery design is a challenging problem. It is a multi-objective decision-making problem not only with respect to technical and economic feasibility but also with respect to environmental impacts, sustainability constraints and limited availability & uncertainties of input data at the early design stage. It is therefore useful to develop a systematic methodology to support the evaluation of processes and the generation of sustainable alternatives for identifying the optimal processing routes. One particular challenge here is to include proactively sustainability analysis as part of the synthesis of biorefinery networks. Another challenge is the handling of several sources of uncertainties such as availability and composition of renewable feedstock, the technical performance of alternative processing technologies and the availability of future markets for biorefinery products, among others.

As part of earlier work in our research group, a systematic methodology to identify/generate optimal biorefineries was developed using the superstructure-based approach, and was implemented in a computer-aided framework. The methodology consists of tools and methods including databases, models, superstructure, and solution strategies to represent, describe and evaluate various combinations of processing networks. The optimization of the network is formulated as a mixed integer nonlinear programming type of problem and solved in GAMS. The methodology was applied for designing optimal biorefinery networks considering biochemical routes. Furthermore, the methodology has also been applied to soybean oil
processing networks and industrial wastewater treatment networks. In the work presented here, the methodology for designing optimal biorefinery networks was expanded with inclusion of thermochemical routes, which means the scope and the size of the biorefinery network problem was extended at the level of the database, the models and the superstructure relevant for thermo-chemical conversion routes (the conversion of biomass feedstocks (corn stover, poplar wood) to fuels and chemicals (FT-gasoline, FT-diesel, bioethanol and higher alcohols) via thermal decomposition processes like pyrolysis and gasification).

In this study, we extend the methodology, models and database by incorporating uncertainty and sustainability analysis as well. Appropriate ranges for uncertain parameters are identified with their correlation/covariance structure and latin hypercube sampling (LHS) is used to sample parameters from their respective domain of uncertainty. The parameter samples are then used as input for solving a deterministic and stochastic optimization problem.

The sustainability analysis was performed in two ways: First, it was performed retrospectively to the optimal biorefinery network solution obtained after the MINLP by using an in-house software (SustainPRO) that employs ICHEME sustainability metrics. Secondly, the sustainability analysis was included proactively as part of the MINLP optimization problem that is performed to find the optimal processing path with respect to multi-criteria assessment including technical, economics and sustainability.

The expanded database and superstructure with uncertainty and sustainability analysis form a powerful process synthesis toolbox to be used in design of future biorefineries with multi-criteria evaluation (technical and economic feasibility, environmental impact and sustainability).

Synthesis and design of optimal biorefinery using an expanded network with thermochemical and biochemical biomass conversion platforms

This study presents the development of an expanded biorefinery processing network for producing biofuels that combines biochemical and thermochemical conversion platforms. The expanded network is coupled to a framework that uses a superstructure based optimization approach to generate and compare of a large number of alternatives at their optimal points. In this study the superstructure for thermochemical conversion route is formulated by using NREL studies of thermochemical conversion of biomass considering 3 biomass feedstocks, 2 products, 3 by-products and 18 processing intervals with combination of 72 processing intervals. This superstructure was integrated with an earlier developed superstructure for biochemical conversion routes thereby forming a formidable number of biorefinery alternatives. The expanded network was demonstrated to be versatile and useful as a decision support tool for identifying at early stage optimal biorefinery concept with respect to technical, economic and environmental criteria.
Synthesis and design of optimal biorefinery using an expanded network with thermochemical and biochemical biomass conversion platforms

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Cheali, P. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
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Event: Poster session presented at 23rd European Symposium on Computer Aided Process Engineering, Lappeenranta, Finland.
Main Research Area: Technical/natural sciences
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Synthesis and Design of Thermochemical and Biochemical Biomass Processing Networks under Uncertainty

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Cheali, P. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
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Main Research Area: Technical/natural sciences
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Systematic Approach for Conceptual Process Design: Production of Styrene From Benzene and Ethylene

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Electrofunctional materials, Copenhagen Business School
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Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences
Electronic versions: Systematic.pdf
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013
Systematic design of tailor-made blended products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. B. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Systematic Design of Tailor-Made Blended Products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
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Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences
Product design, Computer-aided approach, Gasoline, Lubricant
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Systematic Design of Tailor-Made Blended Products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, AstraZeneca
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Pages: 344-368

Systematic substrate adoption methodology (SAM) for future flexible, generic pharmaceutical production processes

The discovery of an effective and safe pharmaceutical product is based on success in clinical trials. Often, several candidate compounds targeting the same disease area are tested in order to identify the most efficacious products. This involves the manufacture of small quantities of compounds (APIs) for early delivery campaigns. Of these candidates only a few will be successful such that further development is required to scale-up the process. Systematic computer-aided methods and tools are required for faster manufacturing of these API candidates. In this work, a substrate adoption methodology (SAM) for a series of substrates with similar molecular functionality has been developed. The objective is to achieve “flexible, fast and future” pharmaceutical production processes by adapting a generic modular process template. Application of the methodology is illustrated through a case study from the pharmaceutical industry. Use of computer-aided methods and tools as part of the methodology is also highlighted.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center, AstraZeneca
Authors: Singh, R. (Intern), Godfrey, A. (Ekstern), Gregertsen, B. (Ekstern), Muller, F. (Ekstern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Pages: 344-368
Systematic sustainable process design and analysis of biodiesel processes

Biodiesel is a promising fuel alternative compared to traditional diesel obtained from conventional sources such as fossil fuel. Many flowsheet alternatives exist for the production of biodiesel and therefore it is necessary to evaluate these alternatives using defined criteria and also from process intensification opportunities. This work focuses on three main aspects that have been incorporated into a systematic computer-aided framework for sustainable process design. First, the creation of a generic superstructure, which consists of all possible process alternatives based on available technology. Second, the evaluation of this superstructure for systematic screening to obtain an appropriate base case design. This is done by first reducing the search space using a sustainability analysis, which provides key indicators for process bottlenecks of different flowsheet configurations and then by further reducing the search space by using economic evaluation and life cycle assessment. Third, the determination of sustainable design with/without process intensification using a phenomena-based synthesis/design method. A detailed step by step application of the framework is highlighted through a biodiesel production case study.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
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ThermoData Engine (TDE) is the first full-scale software implementation of the dynamic data evaluation concept, as reported in this journal. The present paper describes the first application of this concept to the evaluation of thermophysical properties for material streams involving any number of chemical components with assessment of uncertainties. The method involves construction of Redlich-Kister type equations for individual properties (excess volume, thermal conductivity, viscosity, surface tension, and excess enthalpy) and activity-coefficient models for phase equilibrium properties (vapor-liquid equilibrium). Multi-component models are based on those for the pure-components and all binary subsystems evaluated on demand through the TDE software algorithms. Models are described in detail, and extensions to the class structure of the program are provided. Novel program features, such as ready identification of key measurements for subsystems that can reduce the combined uncertainty for a particular stream property, are described. In addition, new product-design features are described for selection of solvents for optimized crystal dissolution, separation of binary crystal mixtures, and solute extraction from a single-component solvent. Planned future developments are summarized.

General information
State: Published
Thermodynamic promotion of carbon dioxide-clathrate hydrate formation by tetrahydrofuran, cyclopentane and their mixtures

Gas clathrate hydrate dissociation pressures are reported for mixtures of carbon dioxide, water and thermodynamic promoters forming structure II hydrates. Hydrate (H)-aqueous liquid (Lw)-vapour (V) equilibrium pressures for the ternary system composed of water, tetrahydrofuran (THF), and carbon dioxide (CO2), with 5.0 mole percent THF in the initial aqueous phase, are presented in the temperature range from 283.3K to 285.2K. At 283.3K, the three-phase equilibrium pressure is determined to be 0.61 MPa (absolute pressure). Four-phase hydrate (H)-aqueous liquid (Lw)-organic liquid (La)-vapour (V) equilibrium data are presented for the ternary system of water-cyclopentane-carbon dioxide at temperatures ranging from 285.2K down to 275.5K. New four-phase H-Lw-La-V equilibrium data for the quaternary system water-THF-cyclopentane-carbon dioxide are presented in the temperature range from 275.1K to 286.6K. It is shown that upon adding THF to the pure aqueous phase to form a 4 mass percent solution, the equilibrium pressure of the formed hydrates may be lowered compared to the ternary system of water, cyclopentane and carbon dioxide. © 2013 Elsevier Ltd.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Computer Aided Process Engineering Center, Ecole Nationale Superieure des Mines
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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
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Scopus rating (2012): SJR 1.302 SNIP 1.987 CiteScore 4.7
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Towards an integrated µ-factory: Integrated micro membrane packed bed reactor

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Bodla, V. (Ekstern), Woodley, J. (Intern), Krühne, U. (Intern), Gernaey, K. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Towards an integrated µ-factory: Design and development of a microfluidic system to include fermentation and biocatalysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Bodla, V. K. (Intern), Woodley, J. (Intern), Krühne, U. (Intern), Gernaey, K. (Intern)
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Towards an integrated µ-factory: Integrated micro membrane packed bed reactor

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Bodla, V. K. (Intern), Woodley, J. (Intern), Krühne, U. (Intern), Gernaey, K. (Intern)
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Event: Abstract from BIOTRANS 2013, Manchester, United Kingdom.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Towards a standardized way of reporting physicochemical data and process metrics for transaminase reactions

Transaminase catalyzed transformations have the potential of becoming a standard tool for the synthesis of optically pure chiral amines [1]. Many studies show the wide span of substrate acceptance and the excellent enantioselectivity that can be achieved [2]. However, many times critical information about the system and the reaction performance is lacking in the otherwise very useful scientific reports at laboratory scale. For instance, although K equilibrium is one of the key determining factors for the design and scale-up any transaminase process, it is very rarely reported [3]. In order to build a broader understanding of the correlation between the underlying physicochemical properties of the system (e.g. substrate
volatility) and the process performance (e.g. gram of product per gram of biocatalyst), it would be highly beneficial if these data were reported, and ideally in a consistent manner. In this poster we will suggest data that preferably should accompany reports on transaminase reactions, and also the underlying motivation for why these data are important.

Towards a standardized way of reporting physicochemical data and process metrics for transaminase reactions

Towards effective biocatalytic process development using microreactor technology

Towards process development for whole cell P450 hydroxylation identifying the bottlenecks using CYP153 as model system

Uncertainty and Sensitivity Analysis on PAT System Performance for Crystallization Processes
Use of continuous lactose fermentation for ethanol production by *Kluveromyces marxianus* for verification and extension of a biochemically structured model

A biochemically structured model has been developed to describe the continuous fermentation of lactose to ethanol by *Kluveromyces marxianus* and allowed metabolic coefficients to be determined. Anaerobic lactose-limited chemostat fermentations at different dilution rates (0.02 – 0.35 h⁻¹) were performed. Species specific rates of consumption/formation, as well as yield coefficients were determined. Ethanol yield (0.655 C-mol ethanol*C-mol lactose⁻¹) was as high as 98 % of theoretical. The modeling procedure allowed calculation of maintenance coefficients for lactose consumption and ethanol production of ms = 0.6029 and me= 0.4218 (C-mol)*(C-mol*h)⁻¹, respectively. True yield coefficients for biomass, ethanol and glycerol production were calculated to be \( Y_{sx}^{true} = 0.114 \), \( Y_{ex}^{true} = 0.192 \) and \( Y_{sg} = 2.250 \) (C-mol)*(C-mol)⁻¹, respectively. Model calculated maintenance and true yield coefficients agreed very closely with those determined by regressions of the experimental data. The model developed provides a solid basis for the rational design of optimised fermentation of cheese whey.

**General information**

State: Published
Organisations: National Food Institute, Division of Industrial Food Research, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Computer Aided Process Engineering Center, Novozymes A/S, University of Calabria
Authors: Sansonetti, S. (Ekstern), Hobley, T. J. (Intern), Curcio, S. (Ekstern), Villadsen, J. (Intern), Sin, G. (Intern)
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- Scopus rating (2015): SJR 2.255 SNIP 1.908 CiteScore 5.47
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 2.41 SNIP 2.104 CiteScore 5.3
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 2.412 SNIP 2.503 CiteScore 5.97
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 2.389 SNIP 2.465 CiteScore 5.25
Use of Water-Oil-Surfactant System Phase Behavior Data/Model for Emulsion-based Chemical Product Design

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2013
Main Research Area: Technical/natural sciences

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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013
Use of 'windows of operation' to guide process design of ω-transaminase catalysed reactions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Lima Ramos, J. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Using micro technology in process screening for improved ω-transaminases

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Ringborg, R. H. (Intern), Krühne, U. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern)
Publication date: 2013
Event: Abstract from International Conference on Implementation of Microreactor Technology into Biotechnology (IMTB2013), Cavtat, Croatia.
Main Research Area: Technical/natural sciences
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Using micro technology in process screening for improved ω-transaminases

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering
Authors: Ringborg, R. H. (Intern), Krühne, U. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern)
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Main Research Area: Technical/natural sciences
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A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes

Process intensification (PI) has the potential to improve existing processes or create new process options, which are needed in order to produce products using more sustainable methods. In principle, an enormous number of process options can be generated but where and how the process should be intensified for the biggest improvement is difficult to identify. In this paper the development of a systematic computer aided model-based synthesis and design methodology incorporating PI is presented. In order to manage the complexities involved, the methodology employs a decomposition-based solution approach. Starting from an analysis of existing processes, the methodology generates a set of process options and reduces their number through several screening steps until from the remaining options, the optimal is found. The application of the methodology is highlighted through a case study involving the chemo-enzymatic synthesis of N-acetyl-d-neuraminic acid (Neu5Ac).

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Achieving process intensification form the application of a phenomena based synthesis, Design and intensification methodology

Process Intensification/Process Systems Engineering.

Process intensification (PI) is a means by which one can achieve a more efficient and sustainable chemical process. Major success in the area of PI has been achieved by Eastman chemicals [1] which in 1984 intensified the process for the manufacture of methyl acetate by replacing with one single reactive distillation column the multi-step process which consisted of one reactor, extractive distillation, liquid-liquid separation and azeotropic distillation. However, except for reactive distillation and dividing wall columns, the implementation of PI still faces challenges [2] because the identification and design of intensified processes is not simple [3]. Lutze et al [3] has developed a systematic PI synthesis/design method at the unit operations (Unit-Ops) level, where the search space is based on a knowledge-base of existing PI equipment. Siirola [4] has proposed a task-based approach known as the means-ends analysis. A limitation with the means-ends analysis is that it becomes difficult to apply if too many corrective tasks should be identified and replaced and if too many alternatives should be considered. From the above PI methods, the starting point is knowledge of existing Unit-Ops and therefore a limitation arising from their application is that they are able to generate new integrations/combinations of intensified equipment but are unable to generate novel PI solutions employing new Unit-Ops. Therefore, incentives exist for a more systematic, efficient and flexible PI methodology covering a wider range of applications which is able to find truly innovative and predictive solutions, not only using knowledge of the existing methods at the Unit-Ops level but also operating at a lower level of aggregation (that is, the phenomena level). This enables the use of apriori knowledge of the Unit-Ops as well as the possibility to design new Unit-Ops. A first version for a phenomena-based synthesis/design (PhenPI) methodology has been developed [5] in which a process flowsheet is generated through the use of involved phenomena such as mixing, phase transition and phase separation [5]. In principle, generating processes from phenomena leads to a large number of process options and therefore, an efficient solution procedure for the evaluation of these process options is needed. To manage this complexity, the PhenPI methodology uses a decomposition based solution approach which breaks down the complex mathematical synthesis/design problem into manageable sub-problems (6 steps). It allows the generation of PI options and their subsequent stepwise reduction of the search space and identification of the best intensified process option. In step-1, the problem definition of the process to be intensified, the process scenario (batch or continuous) and constraints are defined. In step-2, the process is analysed based on the base case design and the flowsheet is converted into a task and phenomena based flowsheet. In step-3, analysis of the process at the task and phenomena level and the use of different tools such as analysis of pure component and mixture properties are used to identify limitations/bottlenecks of the process. From this data, desirable tasks and suitable phenomena are identified to overcome these limitations/bottlenecks and for the processing of tasks in the most efficient manner. In step-4, the involved phenomena are aggregated and/or connected using a set of connectivity rules based on the operating windows of each phenomenon. Based on this, a large number of flowsheet options are generated which are subsequently screened for feasibility by applying logical and structural constraints. In step-5, the remaining flowsheet options are fast screened by constraints for feasibility and for performance using a set of PI performance metrics. The most promising phenomena-based options are transformed into a unit-operation based flowsheet using a set of rules. In step-6, the most promising unit-operation based options from step-5 are optimized in order to identify the best process option. In this paper the PhenPI methodology is presented in detail and highlighted by its application to the production of methyl acetate in order to identify the best PI option with respect to sustainability and other processes requiring reaction-separation processing tasks. It will be shown that the PhenPI methodology systematically not only generates the reactive distillation option proposed by Siirola but also other alternatives which have not been previously considered.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, CHEC Research Centre, Computer Aided Process Engineering Center, H. Lundbeck A/S


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Active pharmaceutical ingredient (API) production involving continuous processes – A process system engineering (PSE)-assisted design framework

A systematic framework is proposed for the design of continuous pharmaceutical manufacturing processes. Specifically, the design framework focuses on organic chemistry based, active pharmaceutical ingredient (API) synthetic processes, but could potentially be extended to biocatalytic and fermentation-based products. The method exploits the synergic combination of continuous flow technologies (e.g., microfluidic techniques) and process systems engineering (PSE) methods and tools for faster process design and increased process understanding throughout the whole drug product and process development cycle. The design framework structures the many different and challenging design problems (e.g., solvent selection, reactor design, and design of separation and purification operations), driving the user from the initial drug discovery steps – where process knowledge is very limited – toward the detailed design and analysis. Examples from the literature of PSE methods and tools applied to pharmaceutical process design and novel pharmaceutical production technologies are provided along the text, assisting in the accumulation and interpretation of process knowledge. Different criteria are suggested for the selection of batch and continuous processes so that the whole design results in low capital and operational costs as well as low environmental footprint. The design framework has been applied to the retrofit of an existing batch-wise process used by H. Lundbeck A/S to produce an API: zuclopenthixol. Some of its batch operations were successfully converted into continuous mode, obtaining higher yields that allowed a significant simplification of the whole process. The material and environmental footprint of the process – evaluated through the process mass intensity index, that is, kg of material used per kg of product – was reduced to half of its initial value, with potential for further reduction. The case-study includes reaction steps typically used by the pharmaceutical industry featuring different characteristic reaction times, as well as L–L separation and distillation-based solvent exchange steps, and thus constitutes a good example of how the design framework can be useful to efficiently design novel or already existing API manufacturing processes taking advantage of continuous processes.
Adaptive Continuous Template-Based Novel Manufacturing Technique for Faster Manufacturing of New APIs for Clinical Trials

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
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Advanced sensitivity and uncertainty analysis for computer-aided process engineering

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A dynamic modelling approach to evaluate GHG emissions from wastewater treatment plants

The widened scope for wastewater treatment plants (WWTP) to consider not only water quality and cost, but also greenhouse gas (GHG) emissions and climate change calls for new tools to evaluate operational strategies/treatment technologies. The IWA Benchmark Simulation Model no. 2 (BSM2) has been widely used within the scientific community for the unbiased comparison of control strategies in wastewater treatment facilities. In this paper, the default set of BSM models is extended with a set of comprehensive dynamic approaches that estimate the most significant on-site (secondary treatment, sludge processing) and off-site (net energy use, embedded chemicals, sludge disposal) sources of GHG emissions. The case study presented here calculates and discusses the changes in the effluent quality (EQI) and operational cost (OCI) indices and the formation of carbon dioxide (CO2), methane (CH4) and nitrous oxide (N2O) when modifying the percentage of total suspended solids (TSS) removal efficiency in the primary clarifier (PRIM). Simulations show that high PRIM efficiency decreases the quantity of TSS entering the activate sludge (AS) section leading to lower operational cost due to better energy recovery (and subsequent reduced GHG emissions) in the sludge line, but increases the overall N2O emissions due to the low C/N ratio as a trade-off. Overloading of the bioreactors as a result of poor PRIM performance: i) increases the biogenic CO2 emissions from BOD oxidation and biomass decay in the AS section; ii) increases off-site CO2 emissions due to higher energy demand during the nitrification stage; and, iii) reduces energy recovery from settled organics. The reported results emphasize the importance of a plant-wide approach and the need to consider the interactions between the different treatment units when evaluating the global warming potential (GWP) of a WWTP. Finally, the paper demonstrates the potential of using the proposed approach as a general model-based tool for determining the most sustainable WWTP operational strategies, which is essential in a water sector where climate change, energy and sustainability are key challenges to be tackled.

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A framework for model-based optimization of bioprocesses under uncertainty: Lignocellulosic ethanol production case

This study presents the development and application of a systematic model-based framework for bioprocess optimization. The framework relies on the identification of sources of uncertainties via global sensitivity analysis, followed by the quantification of their impact on performance evaluation metrics via uncertainty analysis. Finally, stochastic programming is applied to drive the process development efforts forward subject to these uncertainties. The framework is evaluated on four different process configurations for cellulosic ethanol production including Simultaneous Saccharification and Co-Fermentation and Separate Hydrolysis and Co-Fermentation (SSCF and SHCF, respectively) technologies in different operation modes (continuous and continuous with recycle). The results showed that parameters related to pretreatment (e.g. activation energy of the reaction for glucose production, order of reaction, etc.), hydrolysis (inhibition constant for xylose on conversion of cellulose and cellobiose, etc) and co-fermentation (ethanol yield on xylose, inhibition constant on microbial growth, etc.), are the most significant sources of uncertainties affecting the unit production cost of ethanol with a standard deviation of up to 0.13 USD/gal-ethanol. Further stochastic optimization demonstrated the options for further reduction of the production costs with different processing configurations, reaching a reduction of up to 28% in the production cost in the SHCF configuration compared to the base case operation. Further, the framework evaluated here for uncertainties in the technical domain, can also be used to evaluate the impact of market uncertainties (feedstock prices, selling price of ethanol, etc) and political uncertainties (such as subsidies) on the economic feasibility of lignocellulosic ethanol production.
A framework for the design of reacting systems with phase transfer catalysis

A generic modelling framework for phase transition catalyst based reacting systems has been developed and converted into a software tool. The modelling framework accommodates models of different types representing different sub-systems of the PTC-based reactive system; databases of model parameters and carefully collected and checked (for thermodynamic consistency) experimentally measured data. The models, data and software have been tested on various PTC-based reactive systems. Illustrative examples are provided.

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A framework for the design of reacting systems with phase transfer catalysis

A generic modelling framework for phase transition catalyst based reacting systems has been developed and converted into a software tool. The modelling framework accommodates models of different types representing different sub-systems of the PTC-based reactive system; databases of model parameters and carefully collected and checked (for thermodynamic consistency) experimentally measured data. The models, data and software have been tested on various PTC-based reactive systems. Illustrative examples are provided.

General information
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Crystallization processes have a wide range of application as a solid-liquid separation technique in the chemical, the pharmaceutical and the food industries, due to the fact that high quality crystalline products can be produced. The main specifications of the crystal product are usually given in terms of crystal size, size distribution, shape and purity. However, the main difficulty in crystallization processes is to obtain a uniform and reproducible crystal size distribution (CSD). To this end, supersaturation control is often applied to drive the process within the metastable zone in order to enhance the control of the CSD. Although this approach has been shown to produce high quality crystals, the set point operating policies for the controller are usually chosen arbitrarily or by trial-and-error. Therefore a systematic procedure to generate operational policies that guarantee that a targeted CSD can be achieved, can be very useful. For such a procedure to be generic i.e. applicable to many case studies of different chemical systems, it needs to be model-based, preferably linked to a modelling framework with a model generation option to allow a wide application range. Furthermore, for control and monitoring purposes, an appropriate Process Analytical Technology (PAT) system ensuring that the critical process variables are measured and maintained within the design limits also needs to be integrated.

The objectives of this work are to develop a generic systematic design framework for monitoring and control systems applicable to a wide range of crystallization processes and operational scenarios. This framework contains a generic multi-dimensional modelling framework and features for design of operational scenarios and for design of PAT systems. The generality of this approach allows the users to generate a wide range of problem-system specific models through the generic multi-dimensional modelling framework [1]. In order to obtain the desired crystal products, an analytical CSD estimator and a response surface method are employed to generate the operational policy needed to match the desired target CSD. The generated operational policies provide the supersaturation set point and by maintaining the operation at this point, the targeted CSD is achieved. The resulting problem-system specific models and the operational policies become ready for use in model-based design and control/analysis of crystallization operations within a model-based process monitoring and control system (PAT system) [2]. The application of the systematic design framework will be highlighted through a potassium dihydrogen phosphate (KDP) crystallization process case study where the objective is to obtain a desired two-dimensional CSD and crystal shape. Also, integrated visualization tools are used together with the generated data for process control and for product (crystal) property monitoring, illustrating, thereby, the power and unique features of this systematic model-based design procedure.

General information

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A generic process template for continuous pharmaceutical production

In the work reported here, a conceptual generic continuous process template for pharmaceutical production is presented. The template is demonstrated on a nitro reduction case study that should in principle be generic such that it can handle a series of substrates with similar molecular functionality. To assist in adoption of different substrates, a systematic substrate adoption methodology (SAM) has also been developed. The objective of the generic process template together with the SAM is to provide flexibility as well as increased efficiency to continuous processes while reducing inventory for safer operations (from 50 to 100 L in batch or 3 to 5 L in continuous processes). It is shown that the use of the template together with SAM can lead to potential savings in product development times through flexible and efficient production of Kg amounts of product material for clinical trials and other analyses.
A generic process template for continuous pharmaceutical production

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All-Fiber Raman Probe

The design and development of an all-in-fiber probe for Raman spectroscopy are presented in this Thesis. Raman spectroscopy is an optical technique able to probe a sample based on the inelastic scattering of monochromatic light. Due to its high specificity and reliability and to the possibility to perform real-time measurements with little or no sample preparation, Raman spectroscopy is now considered an invaluable analytical tool, finding application in several fields including medicine, defense and process control.

When combined with fiber optics technology, Raman spectroscopy allows for the realization of flexible and minimally-invasive devices, able to reach remote or hardly accessible samples, and to perform in-situ analyses in hazardous environments.

The work behind this Thesis focuses on the proof-of-principle demonstration of a truly in-fiber Raman probe, where all parts are realized by means of fiber components. Assuming the possibility to use a fiber laser with a fundamental radiation at 1064nm, in-fiber efficient second harmonic generation is achieved by optically poling the core of the waveguide delivering the excitation light to the sample. In this way, Raman spectroscopy in the visible range can be performed. The simultaneous delivery of the excitation light and collection of the Raman signal from the sample are achieved by means of a double-clad fiber, whose core and inner cladding act as independent transmission channels. A double-clad fiber coupler allows for the recovery of the collected Raman scattering from the inner-cladding region of the double-clad fiber, thus replacing the bulk dichroic component normally used to demultiplex the pump and Raman signal. A tunable Rayleigh-rejection filter based on a liquid filled-photonic bandgap fiber is also demonstrated in this work.

The integration of the devices described in this Thesis allows for the realization of a complete fiber Raman probe, where also the generation of the excitation radiation is done in-fiber.

General information
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A methodology for cascade selection for co-product removal in the ω-transaminase system

Production of chiral amines using transaminases has indeed been proposed recently as an interesting alternative to conventional methods to help in the synthesis of many new pharmaceuticals. Two reaction strategies have been demonstrated: kinetic resolution and asymmetric synthesis. The latter approach has the advantage that the theoretical yield is 100% compared to 50% for the former [1]. However, a major challenge for asymmetric synthesis is the unfavourable thermodynamic equilibrium for many of the most interesting reactions. Meeting the feasibility criteria that are typical for most pharmaceutical processes can only be achieved by selectively removing the product and/or co-product formed during the reaction (so called in-situ (co)product removal (IS(C)PR)). Several different alternative co-product removal strategies have been suggested, all of which have different impacts on the overall process. Among others, one of the most promising strategies is to use a second enzyme reaction to remove the co-product in an enzymatic cascade [2].

Currently there are no decision tools available to help select appropriate cascade systems for process implementation. In the current work a methodology for choosing a feasible cascade system that will remove co-product to meet process requirements under process relevant conditions will be presented. Decisions are based on thermodynamic constraints, kinetics, selectivity, stability, pH change, cascade enzyme compatibility and downstream processing. The methodology has been applied to an ω-transaminase system which is thermodynamically challenged and enzymatic ISCPR is deployed to shift the equilibrium. The enzymes proposed for co-product removal are dehydrogenases: lactate dehydrogenase (EC 1.1.1.27), alanine dehydrogenase (EC 1.4.1.1), yeast alcohol dehydrogenase (EC 1.1.1.1); pyruvate decarboxylase (EC 4.1.1.1), acetolactate synthase (EC 2.2.1.6) and as co-factor recycling enzymes: glucose dehydrogenase (EC 1.1.1.47), formate dehydrogenase (EC 1.2.1.2) and phosphite dehydrogenase (EC 1.20.1.1). The methodology gives an insight into the constraints of different cascade systems and is the basis for process set-up of selected cascades. Experimental and calculated data will be used to illustrate the methodology.

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References:
A methodology for cascade selection for co-product removal in the ω-transaminase system

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A Model-Based and a Multi-Objective Optimisation Framework for Incremental Scale-Up of Bioreactors

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mauricio Iglesias, M. (Intern), Sin, G. (Intern)
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A model-data based systems approach to process intensification
In recent years process intensification (PI) has attracted much interest as a potential means of process improvement to meet the demands, such as, for sustainable production. A variety of intensified equipment are being developed that potentially creates options to meet these demands. Their developments, however, are largely due to experiment based trial and error approaches and while they do not require validation, they can be time consuming and resource intensive. Also, one may ask, can a truly new intensified unit operation be obtained in this way? An alternative two-stage approach is to apply a model-based synthesis method to systematically generate and evaluate alternatives in the first stage and an experiment-model based validation in the second stage. In this way, the search for alternatives is done very quickly, reliably and systematically over a wide range, while resources are preserved for focused validation of only the promising candidates in the second-stage. This approach, however, would be limited to intensification based on "known" unit operations, unless the PI process synthesis/design is considered at a lower level of aggregation, namely the phenomena level. That is, the model-based synthesis method must employ models at lower levels of aggregation and through combination rules for phenomena, generate (synthesize) new intensified unit operations. An efficient solution procedure for the synthesis problem is needed to tackle the potentially large number of options that would be obtained. Here, established procedures for computer aided molecular design is adopted since combination of phenomena to form unit operations with desired objectives is, in principle, similar to combining atoms to form molecules with desired properties. The concept of the phenomena-based synthesis/design method for process intensification will be presented together with illustrations of its application through case studies. Aspects such as need for models, computer-aided framework, the work-flow and data-flow for the PI synthesis method will also be highlighted.

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A model-data based systems approach to process intensification

In recent years process intensification (PI) has attracted much interest as a potential means of process improvement to meet the demands, such as, for sustainable production. A variety of intensified equipment are being developed that potentially creates options to meet these demands. Their developments, however, are largely due to experiment based trial and error approaches and while they do not require validation, they can be time consuming and resource intensive. Also, one may ask, can a truly new intensified unit operation be obtained in this way? An alternative two-stage approach is to apply a model-based synthesis method to systematically generate and evaluate alternatives in the first stage and an experiment-model based validation in the second stage. In this way, the search for alternatives is done very quickly, reliably and systematically over a wide range, while resources are preserved for focused validation of only the promising candidates in the second-stage. This approach, however, would be limited to intensification based on “known” unit operations, unless the PI process synthesis/design is considered at a lower level of aggregation, namely the phenomena level. That is, the model-based synthesis method must employ models at lower levels of aggregation and through combination rules for phenomena, generate (synthesize) new intensified unit operations. An efficient solution procedure for the synthesis problem is needed to tackle the potentially large number of options that would be obtained. Here, established procedures for computer aided molecular design is adopted since combination of phenomena to form unit operations with desired objectives is, in principle, similar to combining atoms to form molecules with desired properties. The concept of the phenomena-based synthesis/design method for process intensification will be presented together with illustrations of its application through case studies. Aspects such as need for models, computer-aided framework, the work-flow and data-flow for the PI synthesis method will also be highlighted.

A multidisciplinary investigation of a transglutaminase biocatalyst for organic synthesis applications

A New Paradigm for Chemical Engineering?

One of the major concerns facing the world today arises from increasing industrial activities that have lead to rapid depletion of non-renewable resources and increase in pollution. With the current emphasis on sustainability, much improvement is expected from the process industry to minimize raw material, energy usage and waste generation without compromising the economic value of the enterprise. Responding to these challenges requires a new insight into the characteristics of a sustainable system, for example, how to incorporate the product, the process and the related supply chain within the system boundary under investigation? A fundamental rethinking of how to identify the needed chemicals based products and how to design, build and operate the corresponding production units, is necessary. Indeed, the chemical industry today is changed from the chemical industry of forty years ago. Clear evidence of this change comes from the jobs taken by graduating chemical engineering professionals in North America, Europe, and some of the Asian countries. In terms of where the graduating chemical engineers are going to work, a clear shift from the commodity chemical industry to the product oriented businesses has been observed. There is an increasing trend within the chemical industry to focus on products and the sustainable processes that can make them. Do these changes point to a paradigm shift in chemical engineering as a discipline? Historically, two previous paradigm shifts in chemical engineering corresponded to major shifts in chemical engineering as a discipline, which affected not only the education of chemical engineering, but also the development of chemical engineering as a discipline. Has the time come for a new paradigm shift that will prepare the current and future chemical engineering graduates to tackle the complex problems facing the chemicals based industries and serve the modern society more efficiently? The lecture will review the current status of chemical engineering as a discipline, the proposals for the third paradigm, the need for such a paradigm shift and related educational issues.
An integrated knowledge-based framework for synthesis and design of enterprise-wide processing networks

Today chemical processing industries manufacture a wide range of products and provide services that touch billions of people’s lives across the globe in many different ways. Making this requires an effective management of innovation in product and process development. On the other hand, the synthesis and design of processing networks is a complex and multidisciplinary problem, which involves many strategic and tactical decisions at business (considering financial criteria, market competition, supply chain network, etc) and engineering levels (considering synthesis, design and optimization of production technology, its feasibility, sustainability, R&D needs, etc), all of which have a deep impact on the profitability of knowledge based industries. In this talk, an integrated business and engineering framework for synthesis and design of processing network within enterprise wide context is presented. A systematic approach is used to manage the complexity and solving simultaneously both the business and the engineering dimension of the problem. This allows generation and comparison of a large number of alternatives at their optimal point. The result is the identification of the optimal raw material, product portfolio and process technology selection for a given market scenario, their sustainability metrics and risk of investment under market uncertainties enabling risk-aware decision making. The framework is highlighted with successful applications for soybean oil processing (food technology), biorefinery network (renewable chemicals) and wastewater treatment network (petrochemical industry).

An Integrated Methodology for Design of Tailor-Made Blended Products

A computer-aided methodology has been developed for the design of blended (mixture) products. Through this methodology, it is possible to identify the most suitable chemicals for blending, and “tailor” the blend according to specified product needs. The methodology has three stages: 1) product design, 2) process identification, and 3) experimental verification. The principle problem, which is the product design stage is divided into four sub-problems and solved with a decomposition-based approach. In stage two, the ability to produce the chemicals used as building blocks in the blends is analyzed. Finally, experimental work (or detailed model-based verification) is conducted in stage three to validate the selected blend candidates. In this study, the product design stage is highlighted through a case study of gasoline blends with bio-based chemicals. The objective of this study is to identify blended gasoline products that match (or improve) the performance of the conventional gasoline.
An Integrated Methodology for Design of Tailor-Made Blended Products

An important issue for the production of many chemical-based products is related to the future supply of the essential raw materials. Currently, many of these products are derived from fossil fuel based raw materials and from a sustainability point of view, other renewable alternatives need to be considered. In order to achieve this, new products need to be developed by blending the conventional materials with other chemicals that can be produced from renewable resources, such as bio-based chemicals. Blending could offer several advantages, such as, reducing the amount of fossil fuel consumption, decreasing the pollution level and increasing the product safety. In addition, potentially the product attributes also can be improved by blending. However, the product performance may decline when other chemicals are added. In order to maintain/improve the blended product performance, it is necessary to identify the best product blend with the most appropriate chemicals. Therefore, an integrated methodology to design mixture.blend products is developed, which is able to find the most suitable chemicals for blending, and produce blended products that satisfy specific product needs. The methodology has three stages: 1) product design, 2) process identification, and 3) experimental verification. At the first stage, a computer-aided methodology is implemented to quickly identify and evaluate the most promising blend candidates. Subsequently, the ability to produce the chemicals used as the components in the mixtures is analyzed. Finally, experimental work (or detailed model-based verification) is conducted to validate the selected blend candidates. In this paper, the product design issues are highlighted considering only chemicals from known bio-based sources. The product design stage has four tasks. First, the design problem is defined where the product needs are identified, translated into target properties and given target values. Secondly, target property models are retrieved from a property model library developed specifically for this methodology. Thirdly, a mixture.blend design algorithm is applied to obtain the mixtures/blends that match the set of constraints (design targets). This algorithm employs a decomposition based solution strategy to solve the mixture.blend problem. The result is a set of blends that match the constraints, the compositions, values of the target properties and information about their miscibility. Finally, the mixture target property values are verified either with experimental data (if available) or by means of rigorous models for the properties and mixtures that require it. The application of this systematic methodology is highlighted through case studies related to the design of blended gasoline, lubricants and refrigerants, where the objective is to identify blended products that satisfy all the product attributes with at least similar or better performance compared to conventional products.
An Integrated Methodology for Design of Tailor-Made Blended Products: Biofuels and Bio-Based Lubricants

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research › Poster – Annual report year: 2012

An operation protocol for facilitating start-up of single-stage autotrophic nitrogen removing reactors based on process stoichiometry

Start-up and operation of single-stage nitritation/anammox reactor employing complete autotrophic nitrogen can be difficult. Keeping the performance criteria and monitoring the microbial community composition may not be easy or fast enough to take action on time. In this study, a control strategy is developed based on stoichiometric analysis of monitored nitrogen species. This analysis can serve as a strong decision-making tool to take appropriate actions with respect to the operational conditions to accelerate start up or attainment of near complete nitritation-anammox performance.

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mutlu, A. G. (Intern), Vangsgaard, A. K. (Intern), Sin, G. (Intern), Smets, B. F. (Intern)
Number of pages: 5
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Host publication information
Title of host publication: Proceedings of IWA World Water Congress & Exhibition
Main Research Area: Technical/natural sciences
Conference: 2012 IWA World Water Congress and Exhibition, Busan, Korea, Republic of, 16/09/2012 - 16/09/2012
Decision-making, Autotrophic nitrogen removal, Stoichiometry, Anammox
Source: dtu
Source-ID: u::5197
Publication: Research - peer-review › Article in proceedings – Annual report year: 2012
A perspective on PSE in pharmaceutical process development and innovation

The pharmaceutical industry is under growing pressure to increase efficiency, both in production and in process development. This paper discusses the central role of Process Systems Engineering (PSE) methods and tools in pharmaceutical process development and innovation, and searches for answers to questions such as: Which PSE methods can be applied readily? Where is more method development needed? The paper covers key subjects for development of economically and environmentally sustainable pharmaceutical processes, including Process Analytical Technology in its broadest sense, continuous pharmaceutical manufacturing and green processes, and is illustrated with a series of short examples taken from the literature and ongoing research projects.
A phenomena-based methodology for process synthesis incorporating process intensification

General information
State: Published
Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Babi, D. K. (Intern), Woodley, J. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation.
Publication: Research › Paper – Annual report year: 2012

Application of Global Sensitivity Analysis As Preparatory Step for Reduction of a Drying Model of Pharmaceutical Granules

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Ghent University
Application of model uncertainty analysis on the modelling of the drying behaviour of single pharmaceutical granules

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Ghent University
Authors: Mortier, S. (Ekstern), Van Hoey, S. (Ekstern), Cierkens, K. (Ekstern), De Beer, T. (Ekstern), Gernaey, K. (Intern), Nopens, L. (Ekstern)
Publication date: 2012
Event: Abstract from 5th Pan-European QbD & PAT Science Conference, Gent, Belgium.
Main Research Area: Technical/natural sciences
Electronic versions:
C_247_abstract.pdf
Source: dtu
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Application of the UNIFAC-CI Model for Phase Equilibria Predictions of Organic Chemical System

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering
Authors: Mustaffa, A. A. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from InMoTher 2012, Lyon, France.
Main Research Area: Technical/natural sciences
Connectivity index, Property prediction, UNIFAC, Organic systems
Electronic versions:
AZM_InMoTher2012_Abstract.pdf
Source: dtu
Source-ID: u::4262
Publication: Research › Conference abstract for conference – Annual report year: 2012

Architecture evolution of biomass aggregates in single stage nitritation/anammox reactors

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Publication date: 2012
Event: Poster session presented at 14th International Symposium on Microbial Ecology, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
AKV_ISME_poster.pdf

Bibliographical note
Are safe results obtained when SAFT equations are applied to ordinary chemicals?: Part 2: Study of solid–liquid equilibria in binary systems

In a previous work, some irregular behaviours of the PC-SAFT EoS – and more generally of SAFT-type EoS – were pointed out for pure components at low temperatures. In particular, it was shown that for pure fluids at a fixed temperature and pressure, these equations of state were likely to exhibit up to five molar volumes, thus leading to the simultaneous existence of pseudo liquid–liquid and liquid–vapour phase equilibria at a same temperature. In this work, low-temperature calculations are performed using the PC-SAFT EoS which is combined with a fugacity model for the solid phase in order to predict solid–liquid phase equilibria. It is shown that when varying the binary-interaction parameter of the PC-SAFT equation, non-feasible phase diagrams may be calculated including for instance, the presence of a liquid–liquid azeotrope, of a liquid–liquid–solid–solid four-phase equilibrium or the simultaneous existence of several eutectic points.
A robust methodology for kinetic model parameter estimation for biocatalytic reactions

Effective estimation of parameters in biocatalytic reaction kinetic expressions are very important when building process models to enable evaluation of process technology options and alternative biocatalysts. The kinetic models used to describe enzyme-catalyzed reactions generally include several parameters, which are strongly correlated with each other. State-of-the-art methodologies such as nonlinear regression (using progress curves) or graphical analysis (using initial rate data, for example, the Lineweaver-Burke plot, Hanes plot or Dixon plot) often incorporate errors in the estimates and rarely lead to globally optimized parameter values. In this article, a robust methodology to estimate parameters for biocatalytic reaction kinetic expressions is proposed. The methodology determines the parameters in a systematic manner by exploiting the best features of several of the current approaches. The parameter estimation problem is decomposed into five hierarchical steps, where the solution of each of the steps becomes the input for the subsequent step to achieve the final model with the corresponding regressed parameters. The model is further used for validating its performance and determining the correlation of the parameters. The final model with the fitted parameters is able to describe both initial rate and dynamic experiments. Application of the methodology is illustrated with a case study using the x-transaminase catalyzed synthesis of 1-phenylethylamine from acetophenone and 2-propylamine.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Pages: 1186-1196
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Biotechnology Progress
Volume: 28
Issue number: 5
ISSN (Print): 8756-7938
Ratings:
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 2.12 SJR 0.668 SNIP 0.762
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.727 SNIP 0.825 CiteScore 2.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.808 SNIP 0.931 CiteScore 2.2
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
Scopus rating (2004): SJR 0.724 SNIP 0.966
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.736 SNIP 0.944
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.844 SNIP 1.075
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.923 SNIP 1.268
Scopus rating (2000): SJR 0.811 SNIP 1.203
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.012 SNIP 1.267

Original language: English
Biocatalysis, Parameter estimation, Kinetic modeling, Omega-transaminases
DOIs:
10.1002/btpr.1588
Source: dtu
Source-ID: u::4762
A simulation based engineering method to support HAZOP studies

HAZOP is the most commonly used process hazard analysis tool in industry, a systematic yet tedious and time consuming method. The aim of this study is to explore the feasibility of process dynamic simulations to facilitate the HAZOP studies. We propose a simulation-based methodology to complement the conventional HAZOP procedure. The method systematically generates failure scenarios by considering process equipment deviations with pre-defined failure modes. The effect of failure scenarios is then evaluated using dynamic simulations - in this study the K-Spice® software used. The consequences of each failure scenario are summarized using a sensitivity measure, which forms the basis for ranking the significance of failure scenarios. The ranking then reveals the most critical process parameters as well as equipment in a system. The methodology is successfully highlighted using part of gas reinjection process model as case study.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, DONG Energy A/S, Kongsberg Oil & Gas Technologies, Mærsk Oil and Gas A/S
Authors: Enemark-Rasmussen, R. (Ekstern), Cameron, D. (Ekstern), Angelo, P. B. (Ekstern), Sin, G. (Intern)
Pages: 1271-1275
Publication date: 2012

Host publication information
Title of host publication: Proceedings of the 11th International Symposium on Process Systems Engineering
Publisher: Elsevier Science
Editors: Karimi, I., Srinivasan, R.
Series: Computer - Aided Chemical Engineering
Volume: 31
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
HAZOP, Dynamic simulation, Process control, Process model, Safety, Gas-reinjection
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Source-ID: u::4482
Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

Ask the experts: The challenges and benefits of flow chemistry to optimize drug development.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Gernaey, K. (Intern)
Pages: 1780-1781
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Future Medicinal Chemistry
Volume: 4
Issue number: 14
ISSN (Print): 1756-8919
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.953 SNIP 0.763 CiteScore 2.4
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.828 SNIP 0.786 CiteScore 2.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.112 SNIP 0.889 CiteScore 2.46
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.18 SNIP 0.917 CiteScore 2.71
A Systematic Approach for Optimized Water Allocation Through Solution of Large Scale Water/Wastewater Networks Problems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Quaglia, A. (Intern), Pennati, A. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Paper 246e.pdf
Links:
https://aiche.confex.com/aiche/2012/webprogram/Paper278824.html

Bibliographical note
Oral presentation.
Source: dtu
Source-ID: u::5315
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

A Systematic Approach to Controlling the Sewer System

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Urban Water Engineering, Department of Environmental Engineering, Copenhagen Wastewater Innovation
Authors: Mollerup, A. H. (Intern), Mauricio Iglesias, M. (Intern), Mikkelson, P. S. (Intern), Johansen, N. B. (Ekstern), Thorberg, D. (Ekstern), Sin, G. (Intern)
Publication date: 2012

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
System.pdf

Bibliographical note
Title on workshop table of content: Model-Based Analysis of Control Performance in Sewer Systems
Source: orbit
Source-ID: 318552
Publication: Research › Sound/Visual production (digital) – Annual report year: 2012
A systematic methodology for controller tuning in wastewater treatment plants

Wastewater treatment plants are typically subject to continuous disturbances caused by influent variations which exhibit diurnal patterns as well as stochastic changes due to rain and storm water events. In order to achieve an efficient operation, the control system of the plant should be able to respond appropriately and reject these disturbances in the influent. A methodology is described here which systematically addresses the assessment of the plant and the influent dynamics, in order to propose a controller tuning that is best adapted to an existing or planned wastewater treatment plant.

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A systematic methodology for controller tuning in wastewater treatment plants

Wastewater treatment plants are typically subject to continuous disturbances caused by influent variations which exhibit diurnal patterns as well as stochastic changes due to rain and storm water events. In order to achieve an efficient operation, the control system of the plant should be able to respond appropriately and reject these disturbances in the influent. A methodology is described here which systematically addresses the assessment of the plant and the influent dynamics, in order to propose a controller tuning that is best adapted to an existing or planned wastewater treatment plant.
A Systematic Methodology for Design of Emulsion Based Chemical Products

A systematic methodology for emulsion based chemical product design is presented. The methodology employs a model-based product synthesis/design stage and a model-experiment based further refinement and/or validation stage. In this paper only the first stage is presented. The methodology employs a hierarchical approach starting with the identification of the needs to be satisfied by the emulsified product and then building up the formulation by adding one-by-one the different classes of chemicals. A structured database together with dedicated property prediction models and evaluation criteria are employed to obtain a list of formulations that satisfy constraints representing the desired needs (target properties). Through a conceptual case study dealing with the design of a sunscreen lotion, the application of this new methodology is illustrated.

General Information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Pages: 220-224
Publication date: 2012

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Title of host publication: Proceedings of the 11th International Symposium on Process Systems Engineering
Publisher: Elsevier Science
Editors: Karimi, I., Srinivasan, R.
Series: Computer - Aided Chemical Engineering
Volume: 31
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Emulsion, Formulation, Model-base method, product design, Sunscreen
Source: dtu
Source-ID: u::4484
Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

A Systematic Methodology for Design of Emulsion Based Chemical Products

A systems engineering approach to manage the complexity in sustainable chemical product-process design
This paper provides a perspective on model-data based solution approaches for chemical product-process design, which consists of finding the identity of the candidate chemical product, designing the process that can sustainably manufacture it and verifying the performance of the product during application. The chemical product tree is potentially very large and a wide range of options exist for selecting the product to make, the raw material to use as well as the processing route to employ. It is shown that systematic computer-aided methods and tools integrated within a model-data based design framework can manage the complexity associated with product-process problems very efficiently. Three specific computer-aided tools (ICAS, Sustain-Pro and VPPDLab) have
A systems engineering approach to manage the complexity in sustainable chemical product-process design

A two-stage ethanol-based biodiesel production in a packed bed reactor.

A two-stage enzymatic process for producing fatty acid ethyl ester (FAEE) in a packed bed reactor is reported. The process uses an experimental immobilized lipase (NS 88001) and Novozym 435 to catalyze transesterification (first stage) and esterification (second stage), respectively. Both stages were conducted in a simulated series of reactors by repeatedly passing the reaction mixture through a single reactor, with separation of the by-product glycerol and water between passes in the first and second stages, respectively. The second stage brought the major components of biodiesel to ‘in-spec’ levels according to the European biodiesel specifications for methanol-based biodiesel. The highest overall productivity achieved in the first stage was 2.52 kg FAEE(kg catalyst)−1 h−1 at a superficial velocity of 7.6 cm min−1, close to the efficiency of a stirred tank reactor under similar conditions. The overall productivity of the proposed two-stage process was 1.56 kg FAEE(kg catalyst)−1 h−1. Based on this process model, the challenges of scale-up have been addressed and potential continuous process options have been proposed.
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.978 SNIP 0.937
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.068 SNIP 0.987 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.113 SNIP 1.144 CiteScore 2.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.173 SNIP 1.188 CiteScore 3.22
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.255 SNIP 1.312 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.157 SNIP 1.064 CiteScore 2.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.126 SNIP 1.18
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.216 SNIP 1.235
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.136 SNIP 1.265
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.132 SNIP 1.273
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.091 SNIP 1.383
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.162 SNIP 1.369
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.009 SNIP 1.43
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.932 SNIP 1.235
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.817 SNIP 1.052
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.766 SNIP 0.973
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.677 SNIP 0.893
Scopus rating (1999): SJR 0.844 SNIP 1.059

Original language: English
Biodiesel, Lipase, Packed bed reactor, Scale-up
DOIs: 10.1016/j.jbiotec.2012.05.017

Bibliographical note
Source: dtu
Source-ID: u::6434
Benchmarking biological nutrient removal in wastewater treatment plants: influence of mathematical model assumptions

This paper examines the effect of different model assumptions when describing biological nutrient removal (BNR) by the activated sludge models (ASM) 1, 2d & 3. The performance of a nitrogen removal (WWTP1) and a combined nitrogen and phosphorus removal (WWTP2) benchmark wastewater treatment plant was compared for a series of model assumptions. Three different model approaches describing BNR are considered. In the reference case, the original model implementations are used to simulate WWTP1 (ASM1 & 3) and WWTP2 (ASM2d). The second set of models includes a reactive settler, which extends the description of the non-reactive TSS sedimentation and transport in the reference case with the full set of ASM processes. Finally, the third set of models is based on including electron acceptor dependency of biomass decay rates for ASM1 (WWTP1) and ASM2d (WWTP2). The results show that incorporation of a reactive settler: (1) increases the hydrolysis of particulates; (2) increases the overall plant's denitrification efficiency by reducing the SNOx concentration at the bottom of the clarifier; (3) increases the oxidation of COD compounds; (4) increases X\text{ANO}, \text{XOHO}, \text{XPHO}, and X\text{PAO} decay; and, finally, (5) increases the growth of X\text{PAO} and formation of X\text{PAO} for ASM2d, which has a major impact on the whole P removal system. Introduction of electron acceptor dependent decay leads to a substantial increase of the concentration of X\text{ANO}, X\text{OHO}, and X\text{PAO} in the bottom of the clarifier. The paper ends with a critical discussion of the influence of the different model assumptions, and emphasizes the need for a model user to understand the significant differences in simulation results that are obtained when applying different combinations of 'standard' models.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University
Authors: Flores-Alsina, X. (Ekstern), Gernaey, K. V. (Intern), Jeppsson, U. (Ekstern)
Pages: 1496-1505
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Water Science and Technology
Volume: 65
Issue number: 8
ISSN (Print): 0273-1223
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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 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
Calibration and validation of a model describing complete autotrophic nitrogen removal in granular sludge

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Environmental Engineering, Environmental Chemistry, Center for Process Engineering and Technology
Authors: Vangsgaard, A. K. (Intern), Mutlu, A. G. (Intern), Gernaey, K. (Intern), Smets, B. F. (Intern), Sin, G. (Intern)
Pages: 193-194
Publication date: 2012

Host publication information
Title of host publication: Proceedings of IWA Nutrient Removal and Recovery 2012 : Trends in NRR
Main Research Area: Technical/natural sciences
Modeling, Autotrophic nitrogen removal, Anammox, Parameter estimation, Calibration and validation
Source: dtu
Source-ID: u::5175
Publication: Research - peer-review › Article in proceedings – Annual report year: 2012
Carbon dioxide capture processes: Simulation, design and sensitivity analysis

Carbon dioxide is the main greenhouse gas and its major source is combustion of fossil fuels for power generation. The objective of this study is to carry out the steady-state sensitivity analysis for chemical absorption of carbon dioxide capture from flue gas using monoethanolamine solvent. First a consistent simulation of the process verifying a base case design has been performed. Available commercial simulation package Aspen Plus 7.2 is used for the steady state simulations. An
equilibrium based model for the process simulations together with the electrolyte-NRTL model for the vapor liquid equilibrium and associated property models are used. Simulations are performed to investigate the sensitivity of the process variables to change in the design variables including process inputs and disturbances in the property model parameters. Results of the sensitivity analysis on the steady state performance of the process to the L/G ratio to the absorber, CO2 lean solvent loadings, and striper pressure are presented in this paper. Based on the sensitivity analysis process optimization problems have been defined and solved and, a preliminary control structure selection has been made.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Korea Advanced Institute of Science & Technology
Authors: Zaman, M. (Ekstern), Lee, J. H. (Ekstern), Gani, R. (Intern)
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Carbon dioxide capture, Chemical absorption, Sensitivity analysis, Operability and control
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Catalytic aerobic oxidation of bio-renewable chemicals
This thesis covers the investigation of new catalytic systems for the aerobic oxidation of chemicals derived from bio-renewable sources. The effects of different factors and conditions on the reactions were examined. The employed catalysts were characterized by physisorption measurements, SEM, TEM, EDS, XRF and other methods.

Supported gold and ruthenium hydroxide catalyst systems were explored for the aerobic oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDA), a potential polymer building block for the plastic industry, or its dimethyl ester (FDMC). High product selectivities and yields were obtained under optimized conditions.

Heterogeneous catalysts consisting of Au nanoparticles on different supports were shown to efficiently oxidize HMF to FDA or FDMC in water or methanol, respectively. Additionally, the reaction conditions were shown to be adjustable for the exclusive production of intermediate products of the oxidation. Catalysts consisting of Ru(OH)₅ deposited on metal oxide supports, such as, for instance, CeO₂ and MgAl₂O₄, were employed in the aerobic oxidation of HMF in different “green” reaction media, e.g. water and various ionic liquids, under base-free conditions. Moreover, a detailed study on the performance and stability of the ruthenium hydroxide catalysts on magnesium-containing supports under reaction conditions was conducted.

The aerobic oxidation of HMF to form another value-added chemical, 2,5-diformylfuran (DFF), was also investigated with supported Ru(OH)₅ catalysts in organic solvents. The examined catalyst systems and reaction conditions were also shown to be applicable for the efficient oxidation of other substituted furans. Furthermore, novel catalytic systems comprising vanadia supported on zeolites were investigated for the aerobic oxidation of HMF to DFF in organic solvents, and a lixiviation study was performed.

The oxidation of aliphatic alcohols over supported Ru(OH)₅ and RuO₅ catalysts is also described. The highly selective and efficient oxidation of ethanol to acetic acid was shown with supported Ru(OH)₅ and highly dispersed RuO₅ deposited on various metal oxides. Furthermore, this thesis presents the results of the catalytic aerobic oxidative degradation of higher alcohols over supported ruthenium hydroxide catalysts. A very efficient oxidative cleavage of vic-diols to form respective acids was also shown under examined conditions.

Thus, the oxidative transformations of biomass-derived chemicals over different gold and ruthenium-based catalyst systems with oxygen as the abundant oxidant were explored.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Centre for Catalysis and Sustainable Chemistry
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Number of pages: 300
Publication date: 2012

Publication information
Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Catalytic conversion of glycose to 5-hydroxymethylfurfural in ionic liquids: A techno-economic process assessment

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Riisager, A. (Intern), Ståhlberg, T. J. B. (Intern), Fu, W. (Intern), Woodley, J. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Comparison of laser diffraction and image analysis for measurement of Streptomyces coelicolor cell clumps and pellets. Morphology is important in industrial processes involving filamentous organisms because it affects the mixing and mass transfer and can be linked to productivity. Image analysis provides detailed information about the morphology but, in practice, it is often laborious including both collection of high quality images and image processing. Laser diffraction is rapid and fully automatic and provides a volume-weighted distribution of the particle sizes. However, it is based on a number of assumptions that do not always apply to samples. We have evaluated laser diffraction to measure cell clumps and pellets of Streptomyces coelicolor compare to image analysis. Samples, taken five times during fed-batch cultivation, were analyzed by image analysis and laser diffraction. The volume-weighted size distribution was calculated for each sample. Laser diffraction and image analysis yielded similar size distributions, i.e. unimodal or bimodal distributions. Both techniques produced similar estimations of the population means, whereas the estimates of the standard deviations were generally higher using laser diffraction compared to image analysis. Therefore, laser diffraction measurements are high quality and the technique may be useful when rapid measurements of filamentous cell clumps and pellets are required.

General information
State: Published
Organisations: Department of Systems Biology, Center for Microbial Biotechnology, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Technical University of Denmark, Novozymes A/S
Authors: Rønnest, N. P. (Ekstern), Stocks, S. M. (Ekstern), Eliasson Lantz, A. (Intern), Gernaey, K. (Intern)
Pages: 1465-1473
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 1.89 SJR 0.61 SNIP 0.721
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Scopus rating (2015): SJR 0.591 SNIP 0.673 CiteScore 1.66
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.627 SNIP 0.809 CiteScore 1.75
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ISI indexed (2013): ISI indexed yes
Computational Fluid Dynamics at work - Design and Optimization of Microfluidic Applications

Computational Fluid Dynamics (CFD) is presented as a powerful tool to support design and optimization of microfluidic reactors. This is demonstrated by means of three case studies. First a three-dimensional scaffold for tissue engineering purposes is investigated using a combination of CFD and a simple biological model. The result is a suggestion of an improved geometry design. In the second case study a microfluidic cartridge of a novel automated in vitro fertilization device is presented, where the CFD model has supported the fluidic design of the microfluidic network in which the stem cells are grown. In the last case study a biocatalytic microfluidic reactor design is presented in which the material characteristics of substrates and products of the catalytic reaction can be investigated. As model system the transaminase catalyzed formation of methylbenzylamine (MBA) from acetophenone is investigated and it is demonstrated how the experimental investigation along with the CFD model can be used for the characterisation of the performance of the reactor system.
Computational Fluid Dynamics at work - Design and Optimization of Microfluidic Applications

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Smart Biosystems ApS, IVF-SYD, Danish Technological Institute
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Publication date: 2012

Bibliographical note
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Computational Methods Supporting Process Intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Krühne, U. (Intern)
Number of pages: 36
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Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
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Publication: Research › Sound/Visual production (digital) – Annual report year: 2012

Computer-aided approach for design of tailor-made blended products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Computer-aided approach for design of tailor-made blended products

A computer-aided methodology has been developed for the design of blended (mixture) products. Through this methodology, it is possible to identify the most suitable chemicals for blending, and “tailor” the blend according to specified product needs (usually product attributes, e.g. performance as well as regulatory). The product design methodology has four tasks. First, the design problem is defined: the product needs are identified, translated into target properties and the constraints for each target property are defined. Secondly, target property models are retrieved from a property model library developed specifically for this methodology. Thirdly, a mixture/design algorithm is applied to obtain the mixtures/blends (gasoline blend in this case) that match the set of constraints (design targets). The result is a set of blends that match the constraints, the composition of the chemicals present in the blend, values of the target properties and information about their miscibility. Finally, the mixture target property values are verified by means of rigorous models for the properties and mixtures. The application of this systematic methodology is highlighted through case studies related to the design of blended gasoline with different types of blending agents. The objective of this study is to identify blended gasoline products that match the traditional gasoline attributes and identify suitable blending agents for gasoline.

Consistent Prediction of Properties of Systems with Lipids

Equilibria between vapour, liquid and/or solid phases, pure component properties and also the mixture-phase properties are necessary for synthesis, design and analysis of different unit operations found in the production of edible oils, fats and biodiesel. A systematic numerical analysis is employed to determine the needs of phase equilibria and related properties in processes such as Deodorization, Dry Fractionation, Solvent Extraction and Biodiesel Production. Other important use for the data and analysis is in property model development for correct and consistent property prediction. Lipids are found in almost all mixtures involving edible oils, fats and biodiesel. They are also being extracted for use in the pharma-industry.

A database for pure components (lipids) present in these processes and mixtures properties has been developed and made available for different applications (model development, property verification, property prediction, etc.). The database has verified data for fatty acids, acylglycerols, fatty esters, fatty alcohols, vegetable oils, biodiesel and minor compounds as phospholipids, tocopherols, sterols, carotene and squalene, together with a user friendly interface that allows an easy search/retrieve of the data (pure component and mixture properties). In total, there are 240 different pure
compounds, 229 different phase equilibrium systems (72 VLE, 85 LLE, 72 SLE), 63 solid solubility systems, and around 4500 data points on phase equilibria. Critical properties, enthalpy of formation, heats of combustion, heats of fusion, normal melting point, normal boiling point, and also temperature dependent properties such as vapour pressure, liquid enthalpy, heats of vaporization, liquid density, liquid viscosity and surface tension are present. Also the parameters for different well-known thermodynamic models (UNIFAC, UNIQUAC, NRTL) have been added to the database. There is a parameter regression option for those systems for which model parameters have not been reported but experimental data can be found in the database. The available data in literature and the well-known property models have been further extended with group-contribution combined with atom connectivity based models. Some of these models are UNIFAC-CI, PC-SAFT (for pure component properties only) and the NRTL-SAC. In this paper, details of the data available in the database together with an analysis of the data will be presented. The analysis checks for consistency of pure component properties and their use in mixture properties. Thermodynamic consistency tests such as the Van Ness Test, Herrington Test (Area Test), Point Test (Differential Test) and Infinite Dilution Test have also been performed. Based on the analysis, an uncertainty score is given, which is then used to define the weights of data-sets to be used for property model parameter regression. The performance of selected models for pure component properties as well as mixture properties when applied to systems containing lipids will be highlighted.

General information
State: Published
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Publication date: 2012
Event: Abstract from ESAT 2012, Potsdam, Germany.
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation.
Source: dtu
Source-ID: u::5199
Publication: Research › Conference abstract for conference – Annual report year: 2012

Continuous Hydrolysis and Liquid–Liquid Phase Separation of an Active Pharmaceutical Ingredient Intermediate Using a Miniscale Hydrophobic Membrane Separator
Continuous hydrolysis of an active pharmaceutical ingredient intermediate, and subsequent liquid–liquid (L-L) separation of the resulting organic and aqueous phases, have been achieved using a simple PTFE tube reactor connected to a miniscale hydrophobic membrane separator. An alkoxide product, obtained in continuous mode by a Grignard reaction in THF, reacted with acidic water to produce partially miscible organic and aqueous phases containing Mg salts. Despite the partial THF–water miscibility, the two phases could be separated at total flow rates up to 40 mL/min at different flow ratios, using a PTFE membrane with 28 cm² of active area. A less challenging separation of water and toluene was achieved at total flow rates as high as 80 mL/min, with potential to achieve even higher flow rates. The operability and flexibility of the membrane separator and a plate coalescer were compared experimentally as well as from a physical viewpoint. Surface tension-driven L-L separation was analyzed in general terms, critically evaluating different designs. It was shown that microporous membrane L-L separation can offer very large operating windows compared to other separation devices thanks to a high capillary pressure (Laplace pressure) combined with a large number of pores per unit area offering low pressure drop. The separation device can easily be operated by means of a back-pressure regulator ensuring flow-independent separation efficiency. Simple monitoring and control strategies as well as scaling-up/out approaches are proposed, concluding that membrane-based L-L separation may become a standard unit operation for continuous pharmaceutical manufacturing.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, CHEC Research Centre, H. Lundbeck A/S
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Pages: 888-900
Publication date: 2012
Main Research Area: Technical/natural sciences

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Journal: Organic Process Research and Development
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BFI (2018): BFI-level 1
Continuous hydrolysis and L-L phase separation of an active pharmaceutical ingredient using a miniscale PTFE membrane separator

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, CHEC Research Centre, H. Lundbeck A/S
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Event: Abstract from 12th International Conference on Microreaction Technology, Lyon, France.
Main Research Area: Technical/natural sciences
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Publication: Research › Conference abstract for conference – Annual report year: 2012

Controller tuning in wastewater treatment plants

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mauricio Iglesias, M. (Intern), Jørgensen, S. B. (Intern), Sin, G. (Intern)
Number of pages: 28
Publication date: 2012

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Original language: English
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation.
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Publication: Research › Sound/Visual production (digital) – Annual report year: 2012

Control of Process Operations and Monitoring of Product Qualities through Generic Model-based Framework in Crystallization Processes
A generic and systematic model-based framework for the design of a process monitoring and control system to achieve the desired crystal size distribution (CSD) and crystal shape for a wide range of crystallization processes has been developed. This framework combines a generic multi-dimensional modelling framework, tools for design of set point profiles, for design of PAT (Process Analytical Technology) systems as well as option to perform the uncertainty and sensitivity analysis of the PAT system design. Through this framework, it is possible for a wide range of crystallization processes to generate the necessary problem-system specific model, the necessary set point using the extended analytical CSD estimator and the response surface method (RSM) and a PAT system design including implementation of monitoring tools and control strategies in order to produce a desired product with its corresponding target properties. In addition the impact and influence of input uncertainties on the predicted PAT system performance can be quantified, i.e. the risk of not achieving the target specifications of the crystal product can also be investigated. The application of the systematic model-based framework is divided into three sections: a) the application of the generic multi-dimensional modelling framework are highlighted: i) the capability to develop and further extend a batch cooling crystallization model is illustrated through a paracetamol case study, supplemented by a sucrose crystallization example to demonstrate how the framework supports smooth switching between chemical systems with a minimum modelling effort; ii) a potassium dihydrogen phosphate (KDP) case study is used to demonstrate how the model complexity can be increased, that is, by switching from a one-dimensional to a twodimensional description; b) the systematic framework is used in a case study to design a monitoring and control (PAT) system for a potassium dichromate and KDP crystallization processes to achieve the desired target CSD respectively; and c) Based on the PAT system
design in b), the application of uncertainty and sensitivity analysis is then highlighted for the potassium dichromate and KDP crystallization process both in open-loop and closed-loop operation. In the case study, the impact of input uncertainties related to parameters of the nucleation and the crystal growth model on the predicted system performance has been investigated for a one- and two-dimensional CSD and it shown the PAT system design is reliable and robust under considered uncertainties.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Abdul Samad, N. A. F. B. (Intern), Gani, R. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Number of pages: 238
Publication date: 2012

Control of SHARON reactor for autotrophic nitrogen removal in two-reactor configuration
With the perspective of investigating a suitable control design for autotrophic nitrogen removal, this work explores the control design for a SHARON reactor. With this aim, a full model is developed, including the pH dependency, in order to simulate the reactor and determine the optimal operating conditions. Then, the screening of controlled variables and pairing is carried out by an assessment of the effect of the disturbances based on the closed loop disturbance gain plots. Two controlled structures are obtained and benchmarked by their capacity to reject the disturbances before the Anammox reactor.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
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Number of pages: 6
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Publication: Research › Article in proceedings – Annual report year: 2012
Crystallization Kinetics Identification within a Generic Modeling Framework

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Center for Process Engineering and Technology
Authors: Meisler, K. T. (Intern), Abdul Samad, N. A. F. B. (Intern), von Solms, N. (Intern), Gernaey, K. (Intern), Gernaey, K. (Intern)
Number of pages: 2
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences
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Design methodology for bio-based processing: Biodiesel and fatty alcohol production
A systematic design methodology is developed for producing two main products plus side products starting with one or more bio-based renewable source. A superstructure that includes all possible reaction and separation operations is generated through thermodynamic insights and available data. The number of alternative processes is systematically reduced through a screening procedure until only feasible alternatives are obtained. As part of the methodology, process intensification involving reaction-separation tasks is also considered to improve the design by shifting the equilibrium reactions. Economic analysis and net present value are determined to find the best economically and operationally feasible process. The application of the methodology is presented through a case study involving biodiesel and fatty alcohol productions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Chulalongkorn University
Authors: Simasatikul, L. (Ekstern), Arpornwichanop, A. (Ekstern), Gani, R. (Intern)
Pages: 855-859
Publication date: 2012
Main Research Area: Technical/natural sciences
Methodology, Superstructure, Process intensification, Biodiesel, Fatty alcohol production

Bibliographical note
Design of an Emulsified Hand Wash Through a Systematic Model-Based Methodology

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Columbia University
Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences

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Oral presentation.
Source: dtu
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Design of Formulated Products: Experimental Component
A systematic methodology for the design and verification of chemical-based products is proposed. By integrating modeling, and experiments, the search space is efficiently scanned to identify the feasible product candidates. The product design (or verification) problem consists of three stages: computer-aided design (Stage 1), which generates a list of feasible candidates, experimental planning (Stage 2), which generates a list of experiments and checks the available experimental set-ups, and experimental testing (Stage 3), which measures the necessary data and verifies the desirable attributes of the final product. The first stage (Stage 1) has been covered in previous publications, along with detailed case studies. The development of Stage 2 and Stage 3 is considered in this article and highlighted through two case studies involving the design and validation of an insect repellent lotion and a sunscreen lotion.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Gani, R. (Intern), Cheng, Y. S. (Ekstern), Ng, K. M. (Ekstern)
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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
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Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46
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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
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Scopus rating (2010): SJR 1.083 SNIP 1.423
Web of Science (2010): Indexed yes
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Web of Science (2009): Indexed yes
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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
Web of Science (2006): Indexed yes
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Web of Science (2005): Indexed yes
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.694 SNIP 1.578
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.749 SNIP 1.725
Web of Science (2002): Indexed yes
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Web of Science (2001): Indexed yes
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Scopus rating (1999): SJR 1.55 SNIP 1.74

Original language: English
Insect repellent lotion, Product design, Experimental testing, Sunscreen lotion, Formulation design

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Publication: Research - peer-review › Journal article – Annual report year: 2011

Design of microfluidic reactors for biocatalytic reactions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Bodla, V. K. (Intern), Bolic, A. (Intern), Krühne, U. (Intern), Woodley, J. (Intern), Gernaey, K. (Intern)
Development and Analysis of Original UNIFAC-CI and Modified UNIFAC-CI Models for Prediction of VLE and SLE Systems

Prediction of properties is important in chemical process-product design. Group-contribution (GC) methods provide useful tool but there is a need to validate and improve their accuracy when complex chemicals are present in the mixtures. In accordance with that, a combined GC and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties. This so-called GCPlus approach is a hybrid model which combines GC and valence connectivity indices (CI). The main idea is the use of CI to describe the molecular fragmentation that relates properties, the molecular interactions with the molecular structures. One established GC method is the UNIFAC model to predict liquid phase activity coefficients. The needed values of the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, values of the missing GIPs, can be predicted through the GCPlus approach. The predicted values for the GIPs are then used in the UNIFAC model to calculate activity coefficients. In this work, the model parameters for using the GCPlus approach to the original UNIFAC and Modified (Dortmund) UNIFAC have been regressed against vapor-liquid equilibrium (VLE) data and simultaneously against VLE and solid-liquid equilibrium (SLE) data for groups formed by C, H, O, N, Cl and S atoms. Initially the VLE data used to regress those parameters are checked using a quality assessment algorithm which combines four widely used consistency tests (Herington, Van Ness, Point/Differential and Infinite Dilution tests) and also a check on the consistencies of the data with the pure component vapor pressures. The overall quality factors, QVLE obtained for each dataset indicate the quality of each datasets and can then be used as weighting factors, in the objective function for the parameter regression with VLE data (and with SLE data). The performance of the CI-models using parameters regressed against VLE data and simultaneously against VLE and SLE data are compared in terms of the uncertainties of the parameters regressed against the predicted properties and the accuracy of the predictions. In addition, the model performances are compared with their reference UNIFAC models.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Korea University
Authors: Mustaffa, A. A. (Intern), Kontogeorgis, G. (Intern), Kang, J. W. (Ekstern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from 18th Symposium on Thermophysical Properties, Boulder, CO, United States.
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation
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Source-ID: u::4470
Publication: Research › Conference abstract for conference – Annual report year: 2012

Development of continuous pharmaceutical production processes supported by process systems engineering methods and tools

The pharmaceutical industry is undergoing a radical transition towards continuous production processes. Systematic use of process systems engineering (PSE) methods and tools form the key to achieve this transition in a structured and efficient way.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Gernaey, K. (Intern), Cervera Padrell, A. E. (Intern), Woodley, J. (Intern)
Pages: 1371-1374
Publication date: 2012
Main Research Area: Technical/natural sciences
Development of Microbial Transglutaminase for amide bond formation

General information
State: Published
Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, University of Montreal, Universite de Montreal
Authors: T. Gundersen, M. (Intern), Fignolé, K. A. (Ekstern), Pelletier, J. N. (Ekstern)
Publication date: 2012
Event: Poster session presented at biocat 2012, Hamburg, Germany.
Main Research Area: Technical/natural sciences

Development of property models with uncertainty estimate for reliable product-process design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Hukkerikar, A. (Intern), Sarup, B. (Ekstern), Abildskov, J. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2012
Event: Abstract from InMoTher 2012, Lyon, France.
Main Research Area: Technical/natural sciences
Electronic versions: AMH_InMoTher-2012_Abstract.pdf

Bibliographical note
Oral presentation.
Source: dtu
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Publication: Research › Conference abstract for conference – Annual report year: 2012

**Dynamic Effects of Diabatization in Distillation Columns**

The dynamic effects of diabatization in distillation columns are investigated in simulation with primary focus on the heat-integrated distillation column (HIDiC). A generic, dynamic, rst-principle model has been formulated, which is flexible to describe various diabatic distillation configurations. Dynamic Relative Gain Array and Singular Value Analysis have been applied in a comparative study of a conventional distillation column and a HIDiC. The study showed increased input-output coupling due to diabatization. Feasible SISO control structures for the HIDiC were also found. Control-loop feasibility was demonstrated.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Bisgaard, T. (Intern), Huusom, J. K. (Intern), Abildskov, J. (Intern)
Number of pages: 7
Publication date: 2012

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Fluid separation, Distillation columns, Diabatic distillation, Dynamic modeling
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PEC12-42.pdf
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**Dynamic Effects of Diabatization in Distillation Columns**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Bisgaard, T. (Intern)
Number of pages: 16
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**Publication information**
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Main Research Area: Technical/natural sciences
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**Dynamics in population heterogeneity during batch and continuous fermentation of Saccharomyces cerevisiae**

Traditionally, microbial populations in optimization studies of fermentation processes have been considered homogeneous. However, research has shown that a typical microbial population in fermentation is heterogeneous. There are indications that this heterogeneity may be both beneficial (facilitates quick adaptation to new conditions) and harmful (reduces yields and productivities)[1,2]. Typically, gradients of e.g. dissolved oxygen, substrates, and pH are observed in industrial scale fermentation processes. Consequently, microbial cells circulating throughout a bioreactor experience rapid environmental changes, which might pose stress on the cells, affect their metabolism and consequently influence the level of heterogeneity of the population. To gain a deeper understanding of population heterogeneity and the triggering phenomena, a Saccharomyces cerevisiae growth reporter strain based on the expression of green fluorescent protein (GFP) was constructed which enable to perform single cell analysis, and thereby provides a tool to map population
heterogeneity. A factorial design experiment followed by multivariate data analysis demonstrated a highly dynamic behavior with regard to subpopulation distribution during different growth stages. To further simulate which effect gradients have on population heterogeneity, glucose and ethanol perturbations during continuous cultivation were performed. Physiological changes were analyzed on single cell level by using flow cytometry followed by cell sorting of different subpopulations. Furthermore the expression of the reporter gene was examined by qPCR. It could be demonstrated that pulses had a clear influence on population distribution. In conclusion, we now have a tool to study the effect environmental gradients have on population heterogeneity.

General information
State: Published
Organisations: Department of Systems Biology, Center for Microbial Biotechnology, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University, University of Copenhagen
Authors: Heins, A. (Intern), Lencastre Fernandes, R. (Intern), Lundin, L. (Ekstern), Carlquist, M. (Ekstern), Sörensen, S. (Ekstern), Gernaey, K. (Intern), Eliasson Lantz, A. (Intern)
Pages: S199-S200
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Main Research Area: Technical/natural sciences

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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 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
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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
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
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.073 SNIP 1.113
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Publication: Research - peer-review › Editorial – Annual report year: 2012

Editorial note: Best paper of 2010 award

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Purdue University
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Pages: III-IV
Publication date: 2012
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Volume: 40
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 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
Effect of Uncertainties in Physical Property Estimates on Process Design - Sensitivity Analysis

Chemical process design calculations require accurate and reliable physical and thermodynamic property data and property models of pure components and their mixtures in order to obtain reliable design parameters which help to achieve desired specifications. The uncertainties in the property values can arise from the experiments itself or from the property models employed. It is important to consider the effect of these uncertainties on the process design in order to assess the quality and reliability of the final design. The main objective of this work is to develop a systematic methodology for performing sensitivity of process design subject to uncertainties in the property estimates. To this end, first uncertainty analysis of the property models of pure components and their mixtures was performed in order to obtain the uncertainties in the estimated property values. As a next step, sensitivity analysis was performed to evaluate the effect of these uncertainties on the process design. The developed methodology was applied to evaluate the effect of uncertainties in the property estimates on design of different unit operations such as extractive distillation, short path evaporator, equilibrium reactor, liquid-liquid extraction, crystallizer etc. The sensitivity of design parameters to
Uncertainties in the property estimates was performed using one-factor-at-a-time approach. The results showed that depending on the pure components and their mixtures involved, the driving forces they represented, the operating conditions, and the choice of the property prediction models, the input uncertainties resulted in significant uncertainties in the final design. The developed methodology was able to: (i) assess the quality of final design; (ii) identify pure component and mixture properties of critical importance from a process design point-of-view; (iii) identify additional experimentation needs to reduce the most critical uncertainties; and (iv) establish acceptable levels of accuracy for property prediction models employed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CAPEC-PROCESS
Authors: Hukkerikar, A. (Intern), Jones, M. N. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 1
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Event: Abstract from 18th Symposium on Thermophysical Properties, Boulder, CO, United States.
Main Research Area: Technical/natural sciences

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Publication: Research › Conference abstract for conference – Annual report year: 2012

Energibesparende biologisk proces til kvælstoffjernelse i spildevand

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Department of Environmental Engineering, Environmental Chemistry
Authors: Vangsgaard, A. K. (Intern), Gernaey, K. (Intern), Sin, G. (Intern), Mutlu, A. G. (Intern), Smets, B. F. (Intern)
Pages: 16-18
Publication date: 2012
Main Research Area: Technical/natural sciences

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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: Danish
Electronic versions:
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Energy efficiency improvements in energy supply and industry

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre
Authors: Abildskov, J. (Intern), Ahrenfeldt, J. (Intern), Henriksen, U. B. (Intern), Jappe Frandsen, F. (Intern)
Pages: 79-85
Enhancing inhibited fermentations through a dynamic electro-membrane bioreactor

Reverse Electro-Enhanced Dialysis (REED) has been shown to intensify fermentations which are impaired by an ionic product inhibition. Productivity can be greatly enhanced by the in situ product removal from the cultivation broth. The REED process has been tested for different applications, where its strong potential for increasing productivity and product yield has been verified.

REED uses ion exchange membranes and electrical potential gradients to selectively separate the target ion. The main limitation of using membrane separation combined with bioreactors is membrane fouling. REED technology ensures long operation time by reversing periodically the polarity of the imposed electrical field to significantly reduce the influence of membrane fouling. The periodic nature of the electrically driven membrane separation process makes the membrane bioreactor operation non trivial. This challenging operation is associated with different dynamic behaviors of the individual units plus their interaction.

The purpose of this contribution is to show the results of experimental and model based efforts done in order to investigate the operation of a membrane bioreactor. From modeling point of view, it is interesting to reveal to which extend the REED module can facilitate the pH control in the fermenter. In this case, the membrane and reactor unit interactions are exploited to substantially increase the lactate productivity and substrate utilization compared to a conventional fermentation with a crude control of pH.

Experiments using multiple stacks with asynchronical current reversal intervals for improved pH stability were carried out in a bioreactor connected to a REED system. The REED was used for control of the pH process parameter of the bioreactor through exchanging the lactate ions (from lactic acid produced in the bioreactor) with hydroxide ions, which maintained a pH close to optimal growing conditions. The ion-exchange was in turn regulated by a PID control unit, which adjusted the electrical current output between the REED electrodes to match the growing production speed of lactic acid, which increased during the trials as the LAB culture grew in numbers simultaneously.

For the single stack trial, the fluctuations deviate significantly more from the setpoint, compared to the similar setup with multiple stacks operated with dispersed, asynchronical current reversal intervals. For the single stack, no other effect helps to stabilize the pH fluctuations until the current reversal transition has passed and process parameter control is reassessed to bring back the pH to its setpoint. For multiple stacks, the operating stacks immediately respond to the impact of one stack going into current reversal and increase their effect while the single stack recovers. Thereby the deviations are significantly lower, which is preferable, especially when operating with microbial process liquids or continuous process solutions.

Enzyme stability: Process engineering requirements

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Törnvall, U. (Intern), Nordblad, M. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Number of pages: 23
Publication date: 2012
Establishment of a gaseous pH control concept in microbioreactors

Existing methods for pH control in bench-scale bioreactor systems often cannot be directly adapted for microbioreactors. This is because microbioreactors are commonly designed to work with constant volumes, operate bubble-free and have no headspace, which technically rules out any possibility of adding acid/base solution for pH control in microbioreactors. This work reports on the establishment of a gaseous pH control concept in microbioreactors where pH control was achieved by dosing of ammonia (NH₃, 20 000 ppm) and pure carbon dioxide (CO₂) gases to respectively; increase and lower the pH of the reactor content. It encompasses the establishment of an optical pH measurement by means of a fluorescent sensor spot, realization of the necessary gas connections, mixing of gases, and gas-exchange via a thin semi-permeable poly(dimethylsiloxane) (PDMS) membrane. It was shown that addition of NH₃ and CO₂ gases coupled to a simple on/off controller results in a satisfactorily control performance (pH control accuracy = + 0.1 of the set point value and system responses of a few minutes were achieved) within the dynamic measuring range of the optical sensor spot which is between pH 6 and 8.

Estimation of environment-related properties of chemicals for design of sustainable processes: Development of group-contribution+ (GC+) models and uncertainty analysis

The aim of this work is to develop group-3 contribution+ (GC+) method (combined group-contribution (GC) method and atom connectivity index (CI)) based 15 property models to provide reliable estimations of environment-related properties of organic chemicals together with uncertainties of estimated property values. For this purpose, a systematic methodology for property modeling and uncertainty analysis is used. The methodology includes a parameter estimation step to determine parameters of property models and an uncertainty analysis step to establish statistical information about the quality of parameter estimation, such as the parameter covariance, the standard errors in predicted properties, and the confidence intervals. For parameter estimation, large data sets of experimentally measured property values of a wide range of chemicals (hydrocarbons, oxygenated chemicals, nitrogenated chemicals, polyfunctional chemicals, etc.) taken from the database of the US Environmental Protection Agency (EPA) and from the database of USEtox is used. For property modeling and uncertainty analysis, the Marrero and Gani GC method and atom connectivity index method have been considered. In total, 22 environment-related properties, which include the fathead minnow 96-h LC₅₀, Daphnia magna 48-h LC₅₀, oral rat LD₅₀, aqueous solubility, bioconcentration factor, permissible exposure limit (OSHA-TWA), photochemical oxidation potential, global warming potential, ozone depletion potential, acidification potential, emission to urban air (carcinogenic and noncarcinogenic), emission to continental rural air (carcinogenic and noncarcinogenic), emission to continental fresh water (carcinogenic and noncarcinogenic), emission to continental seawater (carcinogenic and noncarcinogenic), emission to continental natural soil (carcinogenic and noncarcinogenic), and emission to continental agricultural soil (carcinogenic and noncarcinogenic) have been modeled and analyzed. The application of the developed property models for the estimation of environment-related properties and uncertainties of the estimated property values is highlighted through an illustrative example. The developed property models provide reliable estimates of environment-related properties needed to perform process synthesis, design, and analysis of sustainable chemical processes and allow one to evaluate the effect of uncertainties of estimated property values on the calculated performance of processes giving useful insights into quality and reliability of the design of sustainable processes.
Estimation of Properties of Pure Components Using Improved Group-Contribution+ (GC+) Based Models and Uncertainty Analysis

Physical and thermodynamic properties of pure components are needed to carry out tasks such as process design and computer aided molecular/mixture design among others. The experimental values of properties of many important pure components have not been measured due to many reasons, and hence they must be estimated. Predictive methods such as the group-contribution+ (GC+) method (combined group-contribution (GC) method and atom connectivity index (CI) method) are generally suitable to estimate the needed property values. For assessing the quality and reliability of the selected property prediction method, an engineer needs to know the uncertainties in the estimated property values obtained from that method. With this information, the engineer can then perform better-informed design calculations by taking into account these uncertainties. Hence, given the importance of reliable estimation of properties and uncertainties in the property estimates in the engineering calculations, this work aims to revise and improve GC+ method based estimation of properties as well as to estimate the confidence intervals of estimated property values. To this end, a systematic methodology for property modeling and uncertainty analysis, in general, is developed and used. In total 21 properties of pure components, which include normal boiling point, critical constants, normal melting point among others have been analysed. The statistical analysis of the model performance for these properties is highlighted through several illustrative examples. Important issues related to property modeling such as thermodynamic consistency of the predicted properties (relation of normal boiling point versus critical temperature etc.) are analysed. The developed methodology is simple, yet sound and effective and provides not only the estimated property values using the GC+ approach, but also the uncertainties in the estimated property values. This feature allows one to evaluate the effects of these uncertainties on the product-process design calculations thereby contributing to better-informed and reliable engineering solutions.

Evaluating the impact of plant-wide WWTP control strategies on energy consumption and greenhouse gas emissions

The objective of this paper is to complement the effluent quality (EQI) and operational cost (OCI) indices used to evaluate (plant-wide) control strategies in wastewater treatment systems with a new dimension dealing with greenhouse gas (GHG) emissions. The GHG evaluation is based on a set of comprehensive dynamic models that estimate the most significant on-site (secondary and sludge treatment, sludge disposal) and off-site (net energy use, embedded chemicals) sources of GHG emissions. The study presented here calculates and discusses the changes in the EQI, OCI and the formation of carbon dioxide (CO2), methane (CH4) and nitrous oxide (N2O) as a consequence of varying four process variables: i) system aeration in the activated sludge section; ii) capture efficiency of particulates in the primary clarifier; iii) the temperature (T) regime in the anaerobic digester; and iv) the control of nitrogen rich returns coming from the sludge treatment. Simulation results show the undesirable effects that energy optimization might have on GHG production: Although off-site CO2 emissions may decrease, primarily as a result of: i) reduced aeration energy requirements; and/or ii) increased energy recovery from the sludge treatment, such effects might be counterbalanced by increased N2O emissions in the activated sludge plant due to the 300-fold stronger greenhouse effect of N2O than CO2. The reported results emphasize the importance of a plant-wide approach and the need to consider the
interactions between the different treatment units when evaluating the global warming potential (GWP) of a wastewater treatment plant.

**General information**

**State:** Published

**Organisations:** Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University, CIT Urban Water Management, Ghent University, Catalan Institute for Water Research, Universite Laval, Sweco Environment, The Water Division of ARCADIS, Black and Veatch

**Authors:** Flores-Alsina, X. (Ekstern), Arnell, M. (Ekstern), Amerlinck, Y. (Ekstern), Corominas, L. (Ekstern), Gernaey, K. (Intern), Guo, L. (Ekstern), Lindblom, E. (Ekstern), Nopens, I. (Ekstern), Porro, J. (Ekstern), Shaw, A. (Ekstern), Snip, L. (Intern), Vanrolleghem, P. A. (Ekstern), Jeppsson, U. (Ekstern)

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

**Electronic versions:**

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**Evaluation of the efficiency of alternative enzyme production technologies**

Enzymes are used in an increasing number of industries. The application of enzymes is extending into the production of lignocellulosic ethanol in processes that economically can compete with fossil fuels. Since lignocellulosic ethanol is based on renewable resources it will have a positive impact on for example the emission of green house gasses. Cellulases and hemicellulases are used for enzymatic hydrolysis of pretreated lignocellulosic biomass, and fermentable sugars are released upon the enzymatic process. Even though many years of research has decreased the amount of enzyme needed in the process, the cost of enzymes is still considered a bottleneck in the economic feasibility of lignocellulase utilization. The purpose of this project was to investigate and compare different technologies for production of these enzymes. The filamentous fungus *Trichoderma reesei* is currently used for industrial production of cellulases and hemicellulases. The aim of the thesiwas to use modeling tools to identify alternative technologies that have higher energy or raw material efficiency than the current technology.

The enzyme production by *T. reesei* was conducted as an aerobic fed-batch fermentation. The process was carried out in pilot scale stirred tank reactors and based on a range of different process conditions, a process model was constructed which satisfactory described the course of fermentation. The process was governed by the rate limiting mass transfer of oxygen from the gas to the liquid phase. During fermentation, filamentous growth of the fungus lead to increased viscosity which hindered mass transfer. These mechanisms were described by a viscosity model based on the biomass concentration of the fermentation broth and a mass transfer correlation that incorporated a viscosity term. An analysis of the uncertainty and sensitivity of the model indicated the biological parameters to be responsible for most of the model uncertainty.

A number of alternative fermentation technologies for enzyme production were identified in the open literature. Their mass transfer capabilities and their energy efficiencies were evaluated by use of the process model. For each technology the scale-up enzyme production was simulated at industrial scale based on equal mass transfer. The technical feasibility of each technology was assessed based on prior knowledge of successful implementation at industrial scale and mechanical complexity of the fermentation vessel. The airlift reactor was identified as a potential high energy efficiency technology for enzyme production with excellent chances of success.

Two different pilot plant configurations of the airlift reactor technology were tested in nine fermentations. The headspace pressure was varied between 0.1 and 1.1 barg and the superficial gas velocity in the airlift riser section was varied between 0.02 and 0.06 m/s. The biological model developed in the stirred tank reactor was shown to apply to the airlift reactor with only small modifications: The mass transfer of oxygen in the airlift reactor was studied and a mass transfer correlation containing the superficial gas velocity and the apparent viscosity of the fermentation broth was shown to describe the experimental data well. The mass transfer rate was approximately 20% lower than the literature data for airlift reactors. Mixing in the pilot scale airlift reactor was also studied. As the mixing time was of the same order of magnitude as the characteristic time for oxygen transfer, mixing could also be limiting the process at that scale. The process model for the airlift reactor was also shown to describe the experimental data well for a range of process conditions.

A cost function for oxygen transfer including the equipment cost and running cost for nutrients and electricity was developed for both the stirred tank reactor and the airlift reactor. The cost function was used to identify an optimum range of reactor configuration and process conditions for industrial scale enzyme production fermentors. It was shown that compared to the stirred tank reactor 22% of the electricity cost might be reduced for the airlift reactor, and the capital cost might also be somewhat lower. However, since the electricity cost is a relatively minor part of the total cost, there might currently not be an obvious fiscal motive to change technology. The cost of nutrients is considerably larger than the electricity cost and was shown to be independent of the technology and process conditions. If the cost structure changes in the future and the airlift reactor is chosen as the alternative production
technology, suggestions on the practical scale-up procedure are given. These include the use of Computational Fluid Dynamics (CFD) and scale-down models of the production environment.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Novozymes A/S  
Authors: Albæk, M. O. (Intern), Gernaey, K. (Intern), Hansen, M. S. (Ekstern), Stocks, S. M. (Ekstern)  
Number of pages: 176  
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Publication: Research › Ph.D. thesis – Annual report year: 2012

**Experiences on dynamic simulation software in chemical engineering education**

Commercial process simulators are increasing interest in the chemical engineer education. In this paper, the use of commercial dynamic simulation software, D-SPICE® and K-Spice®, for three different chemical engineering courses is described and discussed. The courses cover the following topics: basic chemical engineering, operability and safety analysis and process control. User experiences from both teachers and students are presented. The benefits of dynamic simulation as an additional teaching tool are discussed and summarized. The experiences confirm that commercial dynamic simulators provide realistic training and can be successfully integrated into undergraduate and graduate teaching, laboratory courses and research.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Oslo and Akershus University College of Applied Sciences, Technical University of Denmark, Aston University, Kongsberg Oil & Gas Technologies  
Authors: Komulainen, T. M. (Ekstern), Enemark-rasmussen, R. (Ekstern), Sin, G. (Intern), Fletcher, J. P. (Ekstern), Cameron, D. (Ekstern)  
Pages: e153-e162  
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BFI (2017): BFI-level 1  
BFI (2016): BFI-level 1  
Scopus rating (2016): SJR 0.393 SNIP 0.61 CiteScore 0.97  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 0.32 SNIP 0.791 CiteScore 0.75  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 0.364 SNIP 1.009 CiteScore 0.85  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 0.316 SNIP 0.803 CiteScore 0.69  
ISI indexed (2013): ISI indexed no  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 0.973 SNIP 1.778 CiteScore 1.42  
ISI indexed (2012): ISI indexed no
Experimental determination of thermodynamic equilibrium in biocatalytic transamination
The equilibrium constant is a critical parameter for making rational design choices in biocatalytic transamination for the synthesis of chiral amines. However, very few reports are available in the scientific literature determining the equilibrium constant (K) for the transamination of ketones. Various methods for determining (or estimating) equilibrium have previously been suggested, both experimental as well as computational (based on group contribution methods). However, none of these were found suitable for determining the equilibrium constant for the transamination of ketones. Therefore, in this communication we suggest a simple experimental methodology which we hope will stimulate more accurate determination of thermodynamic equilibria when reporting the results of transaminase-catalyzed reactions in order to increase understanding of the relationship between substrate and product molecular structure on reaction thermodynamics.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, University of Graz
Authors: Tufvesson, P. (Intern), Jensen, J. S. (Intern), Kroutil, W. (Ekstern), Woodley, J. M. (Intern)
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Publication date: 2012
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 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
Extending the BSM platform with occurrence, transport and fate of micro-pollutants using the ASM-X framework

The objective of this paper is to demonstrate how occurrence, transport and fate of trace chemicals can be assessed when modelling wastewater treatment plants (WWTP). A modified version of the International Water Association (IWA) Benchmark Simulation Model No 1 (BSM1) used to evaluate control strategies in activated sludge systems is expanded with the ASM-X framework, to describe the behaviour of xenobiotic trace chemicals. In this paper, the capabilities of the BSM – ASM-X combined approach are illustrated with two case studies. First, the occurrence of the antibiotic sulfamethaxole (SMX) is modelled using an influent generator. Administration patterns, bioavailability and body residence time are the basis to generate the user-defined profiles that will describe SMX daily variation patterns in the raw wastewater. Additional simulations also show that transport conditions such as sewer length, oxygen concentration and total suspended solids (TSS) loading might have a strong effect on the concentration and the dynamic behaviour of SMX and its metabolites. The second case study presents the fate of tetracycline (TCY), ciprofloxacin (CIP), diclofenac (DCF) and carbamazepine (CMZ) in the benchmark activated sludge system. The results of these investigations demonstrate that different operating conditions can have opposite effects on the studied compounds, especially when they present co-metabolic/inhibitory behaviour with other substances present in the influent wastewater. Finally, the paper is complemented with: i) a critical discussion of the presented results; ii) a thorough analysis of the limitations of the proposed approach; and, iii) future pathways to improve the overall modelling of trace chemicals.
Extension of computer aided solvent selection and design framework - organic solvents for phase transfer catalysis and solvent selection and solvent mixture design for pharmaceutical applications

Following an Optimal Batch Bioreactor Operations Model

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, University of Colima
Authors: Ibarra-Junquera, V. (Ekstern), Jørgensen, S. B. (Intern), Virgen-Ortiz, J. (Ekstern), Escalante-Minakata, P. (Ekstern), Osuna-Castro, J. (Ekstern)
Pages: 114-128
Publication date: 2012
Main Research Area: Technical/natural sciences

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University
Authors: Flores-Alsina, X. (Ekstern), Plósz, B. (Intern), Lindblom, E. (Ekstern), Gernaey, K. (Intern), Jeppsson, U. (Ekstern)
Number of pages: 8
Publication date: 2012
Main Research Area: Technical/natural sciences
Activated sludge modelling, Benchmarking, Model-based evaluation, Multi-criteria decision making, Organic trace chemicals, Wastewater treatment, Xenobiotics
Source: dtu
Source-ID: u::5241
Publication: Research - peer-review › Paper – Annual report year: 2012

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mitrofanov, I. (Intern), Abildskov, J. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from CHISA 2012, Prague, Czech Republic.
Main Research Area: Technical/natural sciences
Electronic versions:
IGM_CHISA2012_oral_abstract.pdf

Bibliographical note
Oral presentation.
Source: dtu
Source-ID: u::5180
Publication: Research › Conference abstract for conference – Annual report year: 2012

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, University of Colima
Authors: Ibarra-Junquera, V. (Ekstern), Jørgensen, S. B. (Intern), Virgen-Ortiz, J. (Ekstern), Escalante-Minakata, P. (Ekstern), Osuna-Castro, J. (Ekstern)
Pages: 114-128
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering and Processing
Volume: 62
ISSN (Print): 0255-2701
Ratings:
Framework for the analysis of crystallization operations

Crystallization is often applied in the production of salts and/or active pharmaceutical ingredients (API), and the crystallization step is an essential part of the manufacturing process for many chemicals-based products. In recent years, the monitoring and analysis of crystallization operations has received increased attention due to the growing need to control more sophisticated production lines as well as to measure/monitor the final product characteristics.

Crystallization operations involve a combination of several phenomena, and different kinetic models are required for their modeling. Growth of the crystals occurs in multiple dimensions and the relative rates of different growth and other kinetic phenomena control the shape and size distribution of the final product. Including several dimensions in the crystallization will allow a more general description of the kinetic phenomena and the crystallization operation. In order to have a full description of a crystallizer a combination of constitutive (kinetic) models is needed. Development of appropriate...
constitutive models requires data, which for size distributions in crystallization operations is available in the form of chord length distribution data (from Focused Beam Reflectance Measurements (FBRM)). Use of this data for modeling requires a data translation procedure.

The objective of this paper is to present a modeling procedure for systematic development of constitutive models for use in design, analysis and simulation of crystallization operations. This procedure has three main features: a data handling and translation feature, a constitutive model identification feature and a model application feature. For different crystallization operation scenarios, the measured data is translated to create an image of the product. Through the model identification option, the parameters of the constitutive models embedded within the crystallizer model are regressed to match the translated product image. With the models identified, they are applied to understand, design and/or analyze various crystallization operational scenarios.

The paper will present the constitutive model development procedure as part of a general crystallization modeling framework. It will highlight the different features through a case study involving measured data and use it to develop models and finally, the use of the model to analyze different crystallization operations.

**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering

Authors: Meisler, K. T. (Intern), Abdul Samad, N. A. F. B. (Intern), Gernaey, K. (Intern), von Solms, N. (Intern), Gani, R. (Intern)

Publication date: 2012

Event: Abstract from APACT-12, Newcastle, United Kingdom.

Main Research Area: Technical/natural sciences

Source: dtu

Source-ID: u::4277

Publication: Research › Conference abstract for conference – Annual report year: 2012

Full in vitro fertilization laboratory mechanization: toward robotic assisted reproduction?

**Objective:** To describe the current efforts made to standardize different steps of assisted reproductive technology processes by the introduction of new technologies for the nonsubjective sperm selection process, oocyte denudation by mechanical removal of cumulus cells, oocyte positioning, sperm motility screening, fertilization, embryo culture, media replacement by microfluidics, and monitoring of embryo development by time-lapse photography, embryo secretions, and/or O\textsubscript{2} consumption. These technologies could be integrated in a unique and fully automated device.

**Design:** Pubmed database and research and development data from authors.

**Setting:** University-affiliated private center.

**Patient(s):** None.

**Intervention(s):** None.

**Main Outcome Measurement(s):** None.

**Result(s):** Several technologies would be useful for: 1) selection of sperm based on viability; 2) manipulation and removal of the cumulus cells’ narrow channel regions combined with microfluidics; 3) advances in oocyte positioning precision through the use of joystick-controlled micromanipulators; 4) microfluidics allowing the gradual change of a culture medium, which might result in better embryo development as well as reduce the amount of embryo manipulation; 5) time-lapse, proteomic, and metabolic scoring of the developing embryo, allowing multiple and optimized selection of the embryos. The technologies described in this review have not yet reported reliable clinical proofs.

**Conclusion(s):** We already have available some of the technologies described, but we envisage an integrated device, i.e., an IVF lab-on-a-chip, by which oocyte and sperm would be processed to achieve a perfect embryo ready to be delivered into the uterus. With such a device, sample preparation, chemical or biologic reactions, and data collection would be integrated.

**General information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Universidad de Valencia, IVF-SYD

Authors: Meseguer, M. (Ekstern), Krühne, U. (Intern), Laursen, S. (Ekstern)

Pages: 1277-1286

Publication date: 2012

Main Research Area: Technical/natural sciences

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Gernaey, K. (Intern)
Number of pages: 57
Publication date: 2012
Global sensitivity analysis of the BSM2 dynamic influent disturbance scenario generator

This paper presents the results of a global sensitivity analysis (GSA) of a phenomenological model that generates dynamic wastewater treatment plant (WWTP) influent disturbance scenarios. This influent model is part of the Benchmark Simulation Model (BSM) family and creates realistic dry/wet weather files describing diurnal, weekend and seasonal variations through the combination of different generic model blocks, i.e. households, industry, rainfall and infiltration. The GSA is carried out by combining Monte Carlo simulations and standardized regression coefficients (SRC). Cluster analysis is then applied, classifying the influence of the model parameters into strong, medium and weak. The results show that the method is able to decompose the variance of the model predictions (R-2 > 0.9) satisfactorily, thus identifying the model parameters with strongest impact on several flow rate descriptors calculated at different time resolutions. Catchment size (PE) and the production of wastewater per person equivalent (QperPE) are two parameters that strongly influence the yearly average dry weather flow rate and its variability. Wet weather conditions are mainly affected by three parameters: (1) the probability of occurrence of a rain event (Llrain); (2) the catchment size, incorporated in the model as a parameter representing the conversion from mm rain . day(-1) to m(3) . day(-1) (Qpermm); and, (3) the quantity of rain falling on permeable areas (aH). The case study also shows that in both dry and wet weather conditions the SRC ranking changes when the time scale of the analysis is modified, thus demonstrating the potential to identify the effect of the model parameters on the fast/medium/slow dynamics of the flow rate. The paper ends with a discussion on the interpretation of GSA results and of the advantages of using synthetic dynamic flow rate data for WWTP influent scenario generation. This section also includes general suggestions on how to use the proposed methodology to any influent generator to adapt the created time series to a modeller's demands.
Activated sludge modelling, Benchmarking, BSM, Influent modelling, Monte Carlo simulation, Standardized regression coefficients (SRC), Computational Biology, Sanitation, Benchmark Simulation Model BSM mathematical and computer techniques, Monte Carlo simulation mathematical and computer techniques

DOIs:
10.2166/wst.2012.089

Group Contribution+ (GC+) Based Estimation of Environment-Related Properties for Design of Sustainable Processes: Development of Property Models and Uncertainty Analysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S, National Risk Management Research Laboratory
Authors: Hukkerikar, A. (Intern), Sarup, B. (Ekstern), Young, D. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Paper 137a.pdf
Group-contribution* (GC*) based estimation of properties of pure components: Improved property estimation and uncertainty analysis

The aim of this work is to present revised and improved model parameters for group-contribution* (GC*) models (combined group-contribution (GC) method and atom connectivity index (CI) method) employed for the estimation of pure component properties, together with covariance matrices to quantify uncertainties in the estimated property values. For this purpose, a systematic methodology for property modeling and uncertainty analysis of GC models and CI models using maximum-likelihood estimation theory is developed. For parameter estimation, large data-sets of experimentally measured property values of pure components of various classes (hydrocarbons, oxygenated components, nitrogenated components, poly-functional components, etc.) taken from the CAPEC database are used. In total 18 pure component properties are analyzed, namely normal boiling point, critical temperature, critical pressure, critical volume, normal melting point, standard Gibbs energy of formation, standard enthalpy of formation, normal enthalpy of fusion, enthalpy of vaporization at 298 K, enthalpy of vaporization at the normal boiling point, entropy of vaporization at the normal boiling point, flash point, auto ignition temperature, Hansen solubility parameters, Hildebrand solubility parameter, octanol/water partition coefficient, acentric factor, and liquid molar volume at 298 K. Important issues related to property modeling such as reliability and predictive capability of the property prediction models, and thermodynamic consistency of the predicted properties (such as, relation of normal boiling point versus critical temperature) are also analyzed and discussed. The developed methodology is simple, yet sound and effective and provides not only the estimated pure component property values but also the uncertainties (e.g. prediction errors in terms of 95% confidence intervals) in the estimated property values. This feature allows one to evaluate the effects of these uncertainties on product-process design, simulation and optimization calculations, contributing to better-informed and more reliable engineering solutions. (C) 2012 Elsevier B.V. All rights reserved.
Identification of bottlenecks for P450 biotransformation processes

Cytochrome P450 monooxygenases (P450 or CYP) is a group of heme-containing enzymes hydroxylating non-activated hydrocarbons in a stereospecific manner, something that is hard to achieve via classical chemistry. The importance of these reactions can be stressed by the hydroxylation of steroids, but hydroxylation of e.g. alkanes, alcohols and fatty acids are also highly interesting in e.g. the polymer industry if the processes can be designed with high yield and productivity.

The requirement for cofactors, corresponding electron transporting proteins, limited activity and stability of this group of enzymes makes these reactions suitable for whole cell transformations. With the limitations that follow with these requirements it is however a challenging task to reach industrial relevant process targets, especially when it comes to bulk chemicals but also for fine chemicals. Stoichiometric amounts of oxygen and limited water solubility of substrates and products are issues demanding process engineering solutions and if this can be done in parallel with strain development and enzyme engineering it would be optimal. We will present where the current research stands in perspective to an industrial mature P450 biotransformation process identifying the limiting parameters and defining relevant targets.
Identification of bottlenecks for P450 biotransformation processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Andersson, M. T. (Intern), Törnvall, U. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Publication date: 2012
Event: Abstract from biocat 2012, Hamburg, Germany.
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::6312
Publication: Research › Conference abstract for conference – Annual report year: 2012

Immobilization of Escherichia coli containing ω-transaminase activity in LentiKats®
Whole Escherichia coli cells overexpressing ω-transaminase (ω-TA) and immobilized cells entrapped in LentiKats® were used as biocatalysts in the asymmetric synthesis of the aromatic chiral amines 1-phenylethylamine (PEA) and 3-amino-1-phenylbutane (APB). Whole cells were permeabilized with different concentrations of cetrimonium bromide (CTAB) and ethanol; the best results were obtained with CTAB 0.1% which resulted in an increase in reaction rate by 40% compared to the whole cells. The synthesis of PEA was carried out using isopropyl amine (IPA) and L-alanine (Ala) as amino donors. Using whole cell biocatalysis, the reaction with IPA was one order of magnitude faster than with Ala. No reaction was detected when permeabilized E. coli cells containing ω-TA were employed using Ala as the amino donor. Additionally, the synthesis of APB from 4-phenyl-2-butanone and IPA was studied. Whole and permeabilized cells containing ω-TA and their immobilized LentiKats® counterparts showed similar initial reactions rates and yields in the reaction systems, indicating 100% of immobilization efficiency (observed activity/activity immobilized) and absence of diffusional limitations (due to the immobilization). Immobilization of whole and permeabilized cells containing ω-TA in LentiKats® allowed improved stability as the biocatalyst was shown to be efficiently reused for five reaction cycles, retaining around 80% of original activity. © 2012 American Institute of Chemical Engineers Biotechnol. Prog., 2012

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Universidad Autonoma de Barcelona
Pages: 693-698
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Biotechnology Progress
Volume: 28
Issue number: 3
ISSN (Print): 8756-7938
Ratings:
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 2.12 SJR 0.668 SNIP 0.762
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.727 SNIP 0.825 CiteScore 2.07
Web of Science (2015): Indexed yes
Improving productivity and enzyme stability through process design: Lipase catalyzed synthesis of epoxides and esters.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University, Aalborg University
Authors: Hagstrom, A. (Ekstern), Nordblad, M. (Intern), Törnvall, U. (Intern), Woodley, J. (Intern), Hatti-Kaul, R. (Ekstern), Adlercreutz, P. (Ekstern)
Publication date: 2012
Incremental design of control system of SHARON-Anammox process for autotrophic nitrogen removal

With the perspective of investigating a suitable control design for autotrophic nitrogen removal, this work explores the control design for a SHARON-Anammox reactor sequence. With this aim, a full model is developed, including the pH dependency, in order to simulate the reactor and determine the optimal operating conditions. Then, the screening of controlled variables and pairing is carried out by an assessment of the effect of the disturbances based on the closed loop disturbance gain plots. Three control structures are obtained and benchmarked by their capacity to reject the disturbances before the Anammox reactor.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mauricio Iglesias, M. (Intern), Valverde Perez, B. (Intern), Sin, G. (Intern)
Number of pages: 6
Publication date: 2012

Host publication information
Title of host publication: Proceedings of the 10th European Workshop on Advanced Control and Diagnosis
Publisher: Technical University of Denmark (DTU)
Main Research Area: Technical/natural sciences
Conference: 10th European Workshop on Advanced Control and Diagnosis, Kgs. Lyngby, Denmark, 08/11/2012 - 08/11/2012
Electronic versions:
PEC12-59.pdf
Source: dtu
Source-ID: u::5413
Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

Integrated Business and Engineering Framework for Synthesis and Design of Enterprise-Wide Processing Networks

The synthesis and design of processing networks is a complex and multidisciplinary problem, which involves many strategic and tactical decisions at business (considering financial criteria, market competition, supply chain network, etc) and engineering levels (considering synthesis, design and optimisation of production technology, R&D, etc), all of which have a deep impact on the profitability of processing industries. In this study, an integrated business and engineering framework for synthesis and design of processing networks is presented. The framework employs a systematic approach to manage the complexity while solving simultaneously both the business and the engineering aspects of problems, allowing at the same time, comparison of a large number of alternatives at their optimal points. The results identify the optimal raw material, the product portfolio and select the process technology for a given market scenario together with the
optimal material flows through the network and calculate the corresponding performance and sustainability metrics. The framework includes a software infrastructure for integrating different methods and tools needed for problem definition, formulation and solution of the design problem as a MINLP, reducing thereby the time and cost needed to generate and solve the design/synthesis problems and providing efficient data transfer between the tools. A generic structural process model has been implemented within the framework to describe the multidimensional engineering issues allowing thereby fast and flexible model development for various production processes. A case study from vegetable oil industry is used successfully to demonstrate the applicability of the integrated framework for making optimal business and engineering decisions.

**General information**

State: Published  
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S  
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)  
Pages: 213-223  
Publication date: 2012  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Computers & Chemical Engineering  
Volume: 38  
ISSN (Print): 0098-1354  
Ratings:  
BFI (2018): BFI-level 2  
BFI (2017): BFI-level 2  
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  
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
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
Integrating Porous Resins In Enzymatic Processes

Increasing pressure mandated by different government policies, for developing sustainable chemical processes for the synthesis of optically pure compounds, has resulted in increased considerations of biocatalysis as a viable option by many industries. Biocatalysis, with its exquisite selective properties and potential ‘green’ attributes, presents it as a sustainable alternative. Today, the role of biocatalysis is most evident in the pharmaceutical industry and is currently extending towards fine and bulk chemical production as well. The use of hydrolytic enzymes (lipases) is well established in several chemical industries, though certain challenges persist in other types of enzymes (transferases and ketoreductases), thus limiting their implementation in industry. Inhibition by substrate and product as well as low aqueous solubility of substrates has constrained the full potential of these enzymes to be harnessed. Porous resins as opposed to other auxiliary phases, for example organic solvents, are nonbioavailable, biocompatible and offer simpler operational handling (no foaming and emulsification). This strategy has been applied effectively to single substrate – single product systems (oxidation, V microbial degradation and hydrolysis). However, this concept has not been extended to other industrially relevant reactions which are two substrate – two product systems. In this thesis, a methodological framework has been successfully developed to aid in implementing the strategy of integrating porous resins for multi-component systems. In this manner, a generic platform has been established for biocatalytic reactions that require the integration of this strategy.

The framework identifies the key information about the reaction and the process using a step-wise protocol with the required tools. It includes the use of kinetic modelling in characterizing the reaction kinetics, a heuristic approach for screening resins and a model based approach for evaluating the process. Greater knowledge about the enzymatic processes with integrated porous resins can therefore be gained and thus the efficiency of process development with respect to time and resources required (reduced number of experiments) could be increased. Estimating kinetic model parameters for enzymatic reactions is quite complex and frequently leads to identifiability issues. In order to understand the different techniques to estimate the parameters, a number of concepts are discussed in chapter four of this thesis. This knowledge has contributed to the development of a robust methodology for the estimation of kinetic model parameters for biocatalytic reactions, which has also been published in a peer reviewed journal. Screening resins for moderately hydrophobic multi-component systems is challenging. Often it is found that the capacity of the resin is inversely related with product selectivity. Therefore a tradeoff has to be made between these parameters which can be crucial from an economic point of view. A low resin capacity points towards the need for higher resin loading, which in turn determines the equilibrium concentration of the substrate in the reactor and the type of reactor that can be used (stirred tank reactor or packed bed reactor). Similarly low product selectivity would result in higher product concentration in the reactor and thus not aid in alleviating inhibition. Further considerations Process modelling is a very effective tool in evaluating a process. Critical information about the process can be gained by means of simulations, which can further be re-used to tune the reaction or process conditions to harness the full potential of the enzyme. State-of-the-art mathematical techniques for model quality evaluation, such as uncertainty and sensitivity analysis, have been included in this analysis in order to identify the key model parameters for better understanding of the process. Three case studies were used to illustrate the applicability of the methodology to fulfil different objective requirements. The case studies were selected for not only being industrially relevant but as well as having certain limitations which contributed in developing the tools and strategies to overcome them. The asymmetric synthesis of 1-phenylethylamine using -transaminse, the asymmetric synthesis of 1-methyl-3-phenylpropylamine using -transaminse and enantioselective synthesis of 2-octanol using alcohol dehydrogenase were selected. VI of resin stability and cost also have to be taken into account in the screening procedure. The screening therefore becomes...
a multi-objective task that has to be solved simultaneously. Such an approach has been applied in the method formulated in this framework.

To overcome these challenges, different process strategies are required to obtain high yields. A number of different challenges and proposed solutions are discussed in chapter one of this thesis and have also been published as a review. In recent years, integrating porous resins as an auxiliary phase in enzymatic processes, to non-selectively bind the substrate and product as a means to alleviate substrate and product inhibition, has gained considerable recognition. The resins act as a reservoir for the inhibitory substrate and a sink for the inhibitory product and simultaneously attain the required high substrate loading to make the process economically feasible. In this way the potential benefit of the enzyme can be exploited.
Kinetics of acetic acid synthesis from ethanol over a Cu/SiO2 catalyst

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Center for Process Engineering and Technology
Authors: Voss, B. (Intern), Schjødt, N. (Ekstern), Grunwaldt, J. (Intern), Andersen, S. (Ekstern), Woodley, J. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research › Poster – Annual report year: 2012

Lab on a chip automates in vitro cell culturing
A novel in vitro fertilization system is presented based on an incubation chamber and a microfluidic device which serves as advanced microfluidic cultivation chamber. The flow is controlled by hydrostatic height differences and evaporation is avoided with help of mineral oil. Six patient compartments allow six simultaneous temperature and pH controlled cultivations with 12 embryos with continuous logging of the monitoring data. Two media can be controlled with help of opening or closing of openings at the microfluidic disposable devices. The flow rates through the single cell compartments can be controlled up to 20μl/h. A common pH electrode is supplied by 14μl sample, which is expanded with help of DI water.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Università "Magna Graecia" of Catanzaro, Smart Biosystems ApS, Italian Institute of Technology
Authors: Perozziello, G. (Ekstern), Møllenbach, J. (Ekstern), Laursen, S. (Intern), Di Fabrizio, E. (Ekstern), Gernaey, K. (Intern), Krühne, U. (Intern)
Pages: 655-658
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication information
Journal: Microelectronic Engineering
Volume: 98
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Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.69 SJR 0.606 SNIP 0.999
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.533 SNIP 0.856 CiteScore 1.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.592 SNIP 0.897 CiteScore 1.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.602 SNIP 1.001 CiteScore 1.45
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.745 SNIP 0.983 CiteScore 1.44
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.818 SNIP 1.169 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Managing biocatalytic productivity

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Törnvall, U. (Intern), Woodley, J. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Journal article – Annual report year: 2012

Measuring the eco-efficiency of bioprocesses

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Lima Ramos, J. (Intern), Tufvesson, J. (Ekstern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Pages: 9-11
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Communication › Journal article – Annual report year: 2012
Metrics for environmental evaluation of biocatalytic processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Lima Ramos, J. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences

Bibliographical note
Invited lecture.
Publication: Research › Paper – Annual report year: 2012

Model-based analysis of control performance in sewer systems
Design and assessment of control in wastewater systems has to be tackled at all levels, including supervisory and regulatory level. We present here an integrated approach to assessment of control in sewer systems based on modelling and the use of process control tools to assess the controllability of the process. A case study of a subcatchment area in Copenhagen (Denmark) is used to illustrate the combined approach in modelling of the system and control assessment.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Urban Water Engineering, Department of Environmental Engineering, Copenhagen Wastewater Innovation
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Modelbaseret valg og optimering af industrielle bioreaktorer

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Modeling Operating Modes during Plant Life Cycle

Modelling process plants during normal operation requires a set of basic assumptions to define the desired functionalities, which lead to fulfillment of the operational goal(s) for the plant. However, during startup and shutdown as well as during batch operation, an ensemble of interrelated modes are required to cover the whole operational window of a process plant including intermediary operating modes. Development of such an ensemble for a plant would constitute a systematic way of defining the possible plant operating modes and thus provide a platform for also defining a set of candidate control structures. The present contribution focuses on development of a model ensemble for a plant with an illustrative example for a bioreactor.

Starting from a functional model, a process plant may be conceptually designed and qualitative operating models may be developed to cover the different regions within the plant operating window, including transitions between operating regions. Subsequently, qualitative functional models may be developed when the means for achieving the desired functionality are sufficiently specified during the design process. Quantitative mathematical models of plant physics can be used for detailed design and optimization. However, the qualitative functional models already provide a systematic framework based on the notion of means-end abstraction hierarchies. Thereby, functional modeling provides a scientific basis for managing complexity. A functional modeling framework has been implemented to facilitate model development and application in a computer environment. Defining means-end causal relations makes it possible to perform qualitative causal reasoning within a functional modeling framework. Thus, such a framework renders it possible to develop potentially feasible control structures. This ability is based on goal reasoning and development of goal trees from causal relations. These capabilities of functional models extend the application potential of functional modeling significantly beyond that of conventional mathematical modeling representing quantitative physical phenomena. The example case is a continuously operating bioreactor for manufacturing single cell protein from methane, where also the bioreactor start-up is illustrated with switching between operating modes and their associated control structures as seen in a multiloop control configuration.
Modeling Operating Modes for the Monju Nuclear Power Plant

The specification of supervision and control tasks in complex processes requires definition of plant states on various levels of abstraction related to plant operation in start-up, normal operation and shut-down. Modes of plant operation are often specified in relation to a plant decomposition into subsystems or components or defined in relation to phases of the plant process. Multilevel Flow Modeling (MFM) is a methodology for representing goals and functions of complex process plants on multiple levels of means-end abstraction and is based on conceptual distinctions between purposes or goals of the process plant, its function and its structural elements. The paper explains how the means-end concepts of MFM can be used to provide formalized definitions of plant operation modes. The paper will introduce the mode types defined by MFM and show how selected operation modes can be represented for the Japanese fast breeder reactor plant MONJU.
Modelling and control design for SHARON/Anammox reactor sequence

With the perspective of investigating a suitable control design for autotrophic nitrogen removal, this work presents a complete model of the SHARON/Anammox reactor sequence. The dynamics of the reactor were explored pointing out the different scales of the rates in the system: slow microbial metabolism against fast chemical reaction and mass transfer. Likewise, the analysis of the dynamics contributed to establish qualitatively the requirements for control of the reactors, both for regulation and for optimal operation. Work in progress on quantitatively analysing different control structure (pairing of controlled variables with manipulated variables) as well as exploring the feasibility of advanced process control including model predictive control.

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Modelling of physical properties - databases, uncertainties and predictive power
Physical and thermodynamic property in the form of raw data or estimated values for pure compounds and mixtures are important pre-requisites for performing tasks such as, process design, simulation and optimization; computer aided molecular/mixture (product) design; and, product-process analysis. While use of experimentally measured values of the needed properties is desirable in these tasks, the experimental data of the properties of interest may not be available or may not be measurable in many cases. Therefore, property models that are reliable, predictive and easy to use are necessary. However, which models should be used to provide the reliable estimates of the required properties? And, how much measured data is necessary to regress the model parameters? How to ensure predictive capabilities in the developed models? Also, as it is necessary to know the associated uncertainties in the estimated/predicted property values, how to assess the quality and reliability of the estimated/predicted property values?

The paper will review a class of models for prediction of physical and thermodynamic properties of organic chemicals and their mixtures based on the combined group contribution – atom connectivity approach. The development of these models requires measured property data and based on them, the regression of model parameters is performed. Although this class of models is empirical by nature, they do allow extrapolation from the regressed model parameters to predict properties of chemicals not included in the measured data-set. Therefore, they are also considered as predictive models. The paper will highlight different issues/challenges related to the role of the databases and the mathematical and thermodynamic consistency of the measured/estimated data, the predictive nature of the developed models, the uncertainty estimates of the predicted data. Related to the database, the consistency of the collected data, the uncertainties in the measured values, and the amount of data to be used in the regression step, will be discussed and analyzed. Related to modelling, the predictive nature of the models, the calculation of the uncertainties of the estimated property values, the theoretical trends will be illustrated with examples.

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Molecular structure based physical properties modelling

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Monitoring and Control of a Continuous Grignard Reaction for the Synthesis of an Active Pharmaceutical Ingredient Intermediate Using Inline NIR spectroscopy

Inline near-infrared (NIR) spectroscopy has been used to monitor a continuous synthesis of an active pharmaceutical ingredient (API) intermediate by a Grignard alkylation reaction. The reaction between a ketone substrate and allylmagnesium chloride may form significant impurities with excess feeding of the Grignard reagent beyond the stoichiometric ratio. On the other hand, limiting this reagent would imply a loss in yield. Therefore, accurate dosing of the two reactants is essential. A feedforward–feedback control loop was conceived in order to maintain the reaction as closely as possible to the stoichiometric ratio, leading the path to full process automation. The feedback control loop relies on NIR transmission measurements performed in a flow cell where, in contrast to labor-intensive offline HPLC analytical methods, the whole reaction product can be scanned in real time without sample dilution. A robust PLS (projection to latent structures) model was developed with a satisfactory standard error of prediction, providing quantification of the ketone substrate in solutions with a high variability of the major solution component - the alkoxide product. In addition, model performance supervision tools such as the spectral residuals or simple plots of pretreated spectra can assist in the identification of spectral outliers, which in this case could be related to Grignard reagent excess. If the sampling time of the NIR instrument is short enough, manipulating the inputs to the reactor may be used to obtain information about its dynamic behavior. This information is very useful for process control design, assessment of analytical tools and definition of sampling times. In this work, a systematic procedure for chemometric model building is followed, after which a discussion is made on some of the potential applications that can be found when exploiting the fast and rich information provided by NIR spectroscopy.

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Monitoring and control of microbioreactors: An expert opinion on development needs

This perspective article is based on an expert panel review on microbioreactor applications in biochemical and biomedical engineering that was organized by the M3C (measurement, monitoring, modelling and control) Working Group of the European Section of Biochemical Engineering Science (ESBES) in the European Federation of Biotechnology (EFB). The aim of the panel was to provide an updated view on the present status of the subject and to identify critical needs and issues for furthering the successful development of microbioreactor monitoring and control. This will benefit future bioprocess development and in vitro toxicity testing. The article concludes with a set of recommendations for extended use and further development of microbioreactors.

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Multi-enzyme Process Modeling

The subject of this thesis is to develop a methodological framework that can systematically guide mathematical model building for better understanding of multi-enzyme processes. In this way, opportunities for process improvements can be identified by analyzing simulations of either existing or potential process configurations operated under different conditions. In these cases, process engineering, enzyme immobilization and protein engineering are presented as fields that can offer feasible solutions for better process configurations or biocatalyst modification to enhance actual process implementation, especially at an industrial level.

Multi-enzyme processes are characterized by a high degree of complexity due to the mixture of enzymes that catalyze several reactions. Therefore, it is necessary to understand how enzymes act in a coordinated and interactive way, and also how enzymes are affected (in a positive or negative way) by the presence of the other enzymes and compounds in the media.

In this thesis the concept of multi-enzyme in-pot term is adopted for processes that are carried out by the combination of enzymes in a single reactor and implemented at pilot or industrial scale. In order to understand the difference between multi-enzyme processes, a number of concepts are discussed in the second chapter of this thesis and has also been published as a review. Furthermore, a classification of multi-enzyme processes is suggested to clarify the ambiguous definitions found in the scientific literature.

Reliable mathematical models of such multi-catalytic schemes can exploit the potential benefit of these processes. In this way, the best outcome of the process can be obtained understanding the types of modification that are required for process optimization. An effective evaluation of these processes is achieved by applying a methodological framework which provides a systematic way of modeling, a structure, guidance, documentation and support to the modeler. The methodological framework developed here brings many benefits to multienzyme process modeling. This framework identifies generic features of the process and provides the information required to structure the process model by using a step-by-step procedure with the required tools and methods. In this way, this framework increases efficiency of the model design and implementation processes with respect to time and resources needed (fast and effective model development).

Furthermore, this methodology incorporates state-of-the-art methods and provides background and insight into their applications for model development purposes.

The methodological framework, which comprises five steps, is the main result of this thesis. The novel feature of this methodology is the emphasis on the multi-enzyme process concepts that is introduced in all steps. In this way, the most relevant and necessary modeling issues can be precisely identified in order to achieve reliable mathematical structures of the processes. In the same way, specific mathematical techniques, for model quality evaluation such as uncertainty and sensitivity analyses, are included in this methodology. Multienzyme process modeling is tremendously benefited with the introduction of these analyses which mark a big difference in the formulation of reliable models for the multi-enzyme processes. In this way the model parameters that drives the main dynamic behavior can be identified and thus a better understanding of this type of processes.

In order to develop, test and verify the methodology, three case studies were selected, specifically the bi-enzyme process for the production of lactobionic acid, the bi-enzyme process for the production of N-acetyl-D-neuraminic acid, and the tri-enzyme process for the production of 1-phenylethylamine. Furthermore, different capabilities of the methodology are developed due to the valuable contributions of each case study. In this way, the methodology was also proven to be useful for a fast model formulation of multi-enzyme processes. Additionally, programming codes were developed using MATLAB (The Mathworks, Natick, MA) which were also used as computational tools to support the implementation, solution and analysis of all the mathematical problems faced in the case studies.
Multi-scale modeling for prediction of distributed cellular properties in response to substrate spatial gradients in a continuously run microreactor

In large-scale fermentors, non-ideal mixing leads to the development of heterogeneous cell populations. This cell-to-cell variability may explain the differences in e.g. yields for large- and lab-scale cultivations. In this work the anaerobic growth of Saccharomyces cerevisiae in a continuously run microreactor is simulated. A multiscale model consisting of the coupling of a population balance model, a kinetic model and a flow model was developed in order to predict simultaneously local concentrations of substrate (glucose), product (ethanol) and biomass, as well as the local cell size distributions.

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Multi-scale modeling for prediction of distributed cellular properties in response to substrate spatial gradients in a continuously run microreactor

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Neutral lipid accumulation at elevated temperature in conditional mutants of two microalgae species
Triacylglycerols, an energy storage compound in microalgae, are known to be accumulated after nitrogen starvation of microalgae cells. Microalgae could be of importance for future biodiesel production due to their fast growth rate and high oil content. In collections of temperature sensitive mutants of Chlamydomonas reinhardtii and Chlorella vulgaris, nine out of forty-one mutants in C. reinhardtii and eleven out of fifty-three mutants in C. vulgaris contained increased amounts of neutral lipids, predominantly as triacylglycerols. Upon temperature induced cell-cycle arrest, these mutants showed enlarged cellular volume compared with the wild type. The C. reinhardtii mutants were analyzed further and one type of mutants displayed a shift in lipid composition from polar membrane lipids to neutral lipids after a temperature up-shift, while the second type of mutants accumulated more total lipid per cell, predominantly as neutral lipids compared with the wild type. Three C. reinhardtii mutants were analyzed further and found to be arrested after DNA synthesis but prior to cell division in the cell cycle. These mutants will be useful in order to further understand neutral lipid accumulation in microalgae and suggest possibilities for biodiesel production by specific induction of lipid accumulation in microalgal cultures by cell-cycle inhibition.
NIST ThermoData Engine: Extension to Solvent Design and Propagation of Uncertainties for Process Simulation

ThermoData Engine (TDE, NIST Standard Reference Databases 103a and 103b) is the first product that implements the concept of Dynamic Data Evaluation in the fields of thermophysics and thermochemistry, which includes maintaining the comprehensive and up-to-date database of experimentally measured property values and expert system for data analysis and generation of recommended property values at the specified conditions along with uncertainties on demand. The most recent extension of TDE covers solvent design and multi-component process stream property calculations with uncertainty analysis.

Solvent Design function serves three tasks: (1) selection of best solvent for a solid solute, (2) search for a selective solvent for a solid binary mixture, and (3) selection of best solvent for extraction. Solvents are selected from the list of registered compounds encountering more than 27,000 entries. Selection is made by best efficiency (depending on the task, solubility, selectivity, or distribution coefficient, etc.) and matching other requirements requested by the user. At user’s request, efficiency criteria are evaluated based on experimental data for binary mixtures or predictive models (UNIFAC variations). Predictions can be compared to the available experimental data, and uncertainties are estimated for all efficiency criteria. Calculations of the properties of multi-component streams including composition at phase equilibria (flash calculations) are at the heart of process simulation engines. However, the accuracy of such calculations is generally unknown that often leads to overdesign of the operational units and results in significant additional cost. TDE provides a tool for the analysis of uncertainty of property calculations for multi-component streams. A process stream in TDE can be either a pure substance or mixture of chemical compounds under bubble, dew, or specified P-T conditions. VLE compositions and single-phase properties are calculated for process streams. Uncertainties are evaluated with the use of the covariance method where covariance matrices account for experimental uncertainties, curve deviations, and inadequacies of the models. Uncertainty analysis shows relative contributions to the total uncertainty from each component and pair of components.
On controllability of an integrated bioreactor and periodically operated membrane separation process

Investigation of integrated processes involves challenges at both design and control levels, these can mainly be associated with different dynamic behaviors of the individual units plus their interaction. Therefore, the design and operation of the integrated system constitutes a key issue. In order to understand the controlled operation of the integrated process, it is convenient to use a model based approach supported by experimental evidence. Recently, an integrated bioreactor and electrically driven membrane separation process (Reverse Electro-Enhanced Dialysis - REED) has been proposed as a method for intensification of lactic acid fermentation (Rype, 2003). This fermentation has been studied extensively driven by an increasing number of applications of the potential fermentation products. The main limitation of lactic acid bioproduction is that lactic acid bacteria normally are impaired by product inhibition at a certain lactate concentration level. Hence, productivity can be enhanced by the in situ lactate removal from the cultivation broth during pH controlled fermentation. This can be done by means of ion exchange membranes and electrical potential gradients. The novelty of the integrated process lies on the innovative REED technology, where lactate ions are exchanged by hydroxide ions. This allows the lactate removal and simultaneously facilitates the pH control in the fermenter. Long operation time is achieved by reversing periodically the polarity of the imposed electrical field to significantly reduce the influence of membrane fouling. Previously, the REED and fermentation processes have been modeled and investigated separately (Prado-Rubio et al., 2011a; Boonmee, 2003). Additionally, a simple quasi-sequential strategy for integrated process design and control structure development has been proposed (Prado-Rubio et al., 2011b). The main purpose of this first attempt of process integration was to predict the productivity improvements and to reveal to which extend the REED module can facilitate the pH control in the fermenter. There, the membrane and reactor unit interactions are exploited to substantially increase the lactate productivity and substrate utilization compared to a conventional fermentation with a crude control of pH. Nevertheless, the proposed pH control structure is unable to tightly control the pH in the fermenter, which may result in a loss of productivity. The purpose of this contribution is to discuss the controllability of the integrated system, focused on the role of the REED module within the process. Interestingly, there are potential solutions either from process and control structure design such as: i. Account for the productivity enhancement earlier in the integrated process design, ii. Use multiple REED units activated sequentially or iii. Try to avoid the controllers fighting by a more appropriate control structure design. Hopefully merging those ideas, an improved strategy for the integrated process design and control development can be proposed.

One-millilitre microbioreactor with impeller for improved mixing

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Department of Systems Biology, Center for Microbial Biotechnology, Technical University of Denmark
**Operation and Control of Enzymatic Biodiesel Production**

This work explores the control of biodiesel production via an enzymatic catalyst. The process involves the transesterification of oils/fats with an alcohol (usually methanol or ethanol), using enzymatic catalysts to generate mono-alkyl esters (the basis of biodiesel) and glycerol as by-product. Current literature indicates that enzymatic processing of oils and fats to produce biodiesel is technically feasible and developments in immobilization technology indicate that enzyme catalysts can become cost effective compared to chemical processing. However, with very few exceptions, enzyme technology is not currently used in commercial-scale biodiesel production. This is mainly due to non-optimized process designs, which do not use the full potential of the catalysts in a cost-efficient way. Furthermore is it unclear what process variables need to be monitored and controlled to ensure optimal economics. Critical to the project is to develop a control methodology to optimize the productivity of biodiesel production (e.g. the dosing of alcohol to minimize catalyst deactivation, minimization of waste and delivering consistent product quality meeting specifications). For production of biodiesel (BD) via an enzymatic route, batch operation is a straightforward and efficient means for producing BD with its main disadvantage being the downtime between batches. For large-scale production of biodiesel, continuous operation is an attractive alternative as it enables efficient use of manpower and capital assets including equipment and raw materials. Currently our group is evaluating various process configurations for continuous BD production in packed bed reactors (PBRs), continuous stirred tank reactors (CSTRs) and a combination of the aforementioned reactors in series. These configurations will be reviewed to identify the process variables that need to be monitored and controlled.

**Optimal Design of Biodiesel Production Process from Waste Cooking Palm Oil**

A design methodology for biodiesel production from waste cooking palm oil is proposed. The proposed method is flexible to the biodiesel process using various catalyst types: alkali and acid catalyst in homogenous and heterogeneous forms, and different process: enzyme process and supercritical process. A two-step approach of hydrolysis and esterification processes is also considered. Waste cooking palm oil consists of a mixture of triglyceride (e.g., trilaurin, tripalmitin, triolein, tristearin, trilinolein and trilinolenin) and free fatty acids (e.g., lauric acid, palmitic acid, stearic acid, oleic acid, linoleic and linolenic acid). A driving force approach and thermodynamic insight are employed to design separation units (e.g., flash separator and distillation) minimizing the energy consumption. Steady-state simulations of the developed biodiesel processes are performed and economic analysis is used to find a suitable biodiesel process. The results show that based on a net present value, the heterogeneous acid catalyzed process is the best process for biodiesel production. With the design methodology, the proposed biodiesel process can save the energy requirement of 41.5%, compared with a conventional process.
Optimization based tuning approach for offset free MPC

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for multivariate processes that can be represented by an ARX model. The advantage of ARX model representations is that standard system identification techniques using convex optimization can be used for identification of such models from input-output data. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The ARMAX model description resulting from the extension can be realized as a state space model in innovation form. The MPC is designed and implemented based on this state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop expressions these evaluations can be done relatively quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure. The method is demonstrated on two simulated examples: A Wood-Berry distillation column example and a cement mill example.

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PAT tools for fermentation processes
The publication of the Process Analytical Technology (PAT) guidance has been one of the most important milestones for pharmaceutical production during the past ten years. The ideas outlined in the PAT guidance are also applied in other industries, for example the fermentation industry. Process knowledge is central in PAT projects. This manuscript therefore gives a brief overview of a number of PAT tools for collecting process knowledge on fermentation processes: on-line sensors, mechanistic models and small-scale equipment for high-throughput experimentation. The manuscript ends with a short perspective on future developments.

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PAT tools for fermentation processes

The publication of the Process Analytical Technology (PAT) guidance has been one of the most important milestones for pharmaceutical production during the past ten years. The ideas outlined in the PAT guidance are also applied in other industries, for example the fermentation industry. Process knowledge is central in PAT projects. This presentation therefore gives a brief overview of a number of PAT tools for collecting process knowledge on fermentation processes:

- On-line sensors, where for example spectroscopic measurements are increasingly applied
- Mechanistic models, which can be used to summarize process knowledge, to support experimental work, and also within design of PAT systems
- Small-scale equipment for high-throughput experimentation, a field which has been researched intensively during the past decade

The presentation ends with a short perspective on future developments
Phase equilibrium modeling of gas hydrate systems for CO2 capture

Two thermodynamic models capable of describing dissociation pressures of mixed gas clathrate hydrates formed from ternary mixtures of CO2, N2 and liquid water, are presented. Both of the models utilize the Cubic-Plus-Association (CPA) equation of state (EOS) for the thermodynamic description of the non-solid phases (vapor and liquid). The solid hydrate phase is described by the van der Waals–Platteeuw model as presented by Parrish and Prausnitz. An algorithm for combining the CPA EOS with the van der Waals–Platteeuw model in a calculation of hydrate dissociation pressure is presented. Two models are described in this work. They differ in their method for describing the Langmuir adsorption coefficients in the van der Waals–Platteeuw model. These models are named Model I and Model II. Model I utilizes a statistical thermodynamics approach based on Lennard-Jones–Devonshire theory, using the spherical core Kihara cell potential. Model II uses a two-parameter explicit expression for the Langmuir adsorption coefficient, based on Langmuir adsorption theory. With two hydrate formers, four parameters in the Kihara cell potentials are fitted for Model I. Sixteen parameters are required to be fitted for Model II. The two model parameter sets are fitted to pure hydrate dissociation pressures and mixed hydrate dissociation pressures found in literature. In the fitting process, vapor phases with initial mole fractions of CO2 below 0.15 are assumed to form structure II hydrates, while structure I hydrates are assumed to form from vapor phases with initial mole fractions of CO2 at or above 0.15. The two models are validated against mixed hydrate equilibrium data found in literature. Both dissociation pressures and hydrate compositions are considered in the validation process. With the fitted parameters, Model I predicts a hydrate structure transition from structure II hydrates at vapor phase mole fractions of CO2 below 0.12 to 0.16 (depending on temperature) to structure I hydrates at mole fractions of CO2 above this concentration range. The exact transition concentration is shown to increase with increasing temperature. Model II predicts structure I hydrates to be stable in concentrations down to vapor phase mole fractions of CO2 in the order of 0.001 to 0.02, depending on temperature. Model II predicts the transition concentration to decrease with increasing temperature. Since there is disparity amongst the different literature data for this system, it was not possible to determine unequivocally, which of the two models perform better.
pH control structure design for a periodically operated membrane separation process

A bioreactor integrated with an electrically driven membrane separation process (Reverse Electro-Enhanced Dialysis – REED) is under investigation as potential technology for intensifying lactic acid bioproduction. In this contribution the pH regulation issue in the periodically operated REED module is studied. A methodology for control structure design is proposed to handle the dynamic system. A sensitivity analysis is used for the conceptual design of the control structure. Dynamic simulations are employed to evaluate the sensitivity index. From the analysis a periodic input-resetting control structure is selected. The system controls pH using the imposed current density and resets the current density manipulating the hydroxide inlet concentration to the dialysate channel. The control structure is satisfactorily achieving a desired pH at the outlet of the feed channel in REED from period to period and resetting the current density. Thus suitable performance is achieved within a large part of the operating window.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Membrane Technology group
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Phenomena-based Process Synthesis and Design to achieve Process Intensification

Process intensification (PI) has the potential to improve existing processes, necessary to achieve a more sustainable production. PI can be achieved at different levels. That is, the unit operations, functional and/or phenomena level. The highest impact is expected by looking at processes at the lowest level of aggregation: phenomena. Therefore, in this paper, a phenomena-based synthesis/design methodology is presented. Using this methodology, a systematic identification of necessary and desirable (integrated) phenomena as well as generation and screening of phenomena-based flowsheet options are made using a decomposition based solution approach. The developed methodology is highlighted through a case study involving the production of isopropyl-acetate.

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Babi, D. K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
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Methodology, Phenomena, Process synthesis, Process intensification

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pH variation and influence in a nitrogen converting biofilm

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Vangsgaard, A. K. (Intern), Mauricio Iglesias, M. (Intern), Valverde Perez, B. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)
Pages: 15-16
Publication date: 2012

Physiological heterogeneities in microbial populations and implications for physical stress tolerance

Background: Traditionally average values of the whole population are considered when analysing microbial cell cultivations. However, a typical microbial population in a bioreactor is heterogeneous in most phenotypes measurable at a single-cell level. There are indications that such heterogeneity may be unfavourable on the one hand (reduces yields and productivities), but also beneficial on the other hand (facilitates quick adaptation to new conditions - i.e. increases the robustness of the fermentation process). Understanding and control of microbial population heterogeneity is thus of major importance for improving microbial cell factory processes.

Results: In this work, a dual reporter system was developed and applied to map growth and cell fitness heterogeneities within budding yeast populations during aerobic cultivation in well-mixed bioreactors. The reporter strain, which was based on the expression of green fluorescent protein (GFP) under the control of the ribosomal protein RPL22a promoter, made it possible to distinguish cell growth phases by the level of fluorescence intensity. Furthermore, by exploiting the strong correlation of intracellular GFP level and cell membrane integrity it was possible to distinguish subpopulations with high and low cell membrane robustness and hence ability to withstand freeze-thaw stress. A strong inverse correlation between growth and cell membrane robustness was observed, which further supports the hypothesis that cellular resources are limited and need to be distributed as a trade-off between two functions: growth and robustness. In addition, the trade-off was shown to vary within the population, and the occurrence of two distinct subpopulations shifting between these two antagonistic modes of cell operation could be distinguished.

Conclusions: The reporter strain enabled mapping of population heterogeneities in growth and cell membrane robustness towards freeze-thaw stress at different phases of cell cultivation. The described reporter system is a valuable tool for understanding the effect of environmental conditions on population heterogeneity of microbial cells and thereby to understand cell responses during industrial process-like conditions. It may be applied to identify more robust subpopulations, and for developing novel strategies for strain improvement and process design for more effective bioprocessing.

General information
State: Published
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Process considerations for protein engineering of ω-Transaminase

Over the past decades, the use of biocatalysis in the chemical and pharmaceutical industry has significantly increased. In parallel and contributing to this trend, many enzymes have been discovered and isolated from different biological sources. This has broadened the scope of biocatalysis and nowadays allows the green regio- and enantio-selective synthesis of many compounds, potentially with less time and energy demand and avoiding the use of toxic reagents. The technology therefore has many advantages over classical chemical synthesis to prepare fine chemical and pharmaceutical intermediates.

However, often wild type enzyme does not fit the requirements of the process conditions, where high substrate and product concentrations as well as high productivity demands of the catalyst (g product per g biocatalyst), are key to economic feasibility. The question thus arises whether to fit the process to the catalyst or the other way around. Modern biotechnology has indeed seen a tremendous development in the last decades which in fact makes it possible to improve many of the enzyme properties needed, such as, tolerance to pH and temperature, substrate and product inhibition and finally the enantio specificity (e.e). However, it is critical that this is done in parallel process development to make sure that the properties developed also fit the process requirements.

As an example, ω-transaminases (EC 2.6.1.18) can be used to produce optically pure chiral amines (with 100% theoretical yield) which are important building blocks for the chemical and pharmaceutical industries. On the other hand, there are a number of challenges associated with the use of this enzyme for instance substrate and product inhibition, and a potentially unfavorable equilibrium.

In the present work it was investigated how changes to a wild type transaminase through protein engineering changed the characteristics of the biocatalyst and the implications this would have on a process. A methodology for characterizing the biocatalyst was developed which was subsequently applied to the wild type and 5 mutants selected. It was seen that the mutants had a better tolerance to the substrate and to higher temperature as well as displaying a broader pH tolerance. Based on the improved properties it could be shown that the feasibility of the process was significantly improved and that these properties opened up the potential for improvements in the process, such as operating at a higher pH for facilitated in-situ product removal.
Process Design and Evaluation for Chemicals Based on Renewable Resources

One of the key steps in process design is choosing between alternative technologies, especially for processes producing bulk and commodity chemicals. Recently, driven by the increasing oil prices and diminishing reserves, the production of bulk and commodity chemicals from renewable feedstocks has gained considerable interest. Renewable feedstocks usually cannot be converted into fuels and chemicals with existing process facilities due to the molecular functionality and variety of the most common renewable feedstock (biomass). Therefore new types of catalytic methods as well as new types of processes for converting renewable feedstocks to bulk and commodity chemicals are required. In the future, it seems increasingly likely that a combination of biocatalysts (in the form of enzymes) as well as chemical catalysts will be needed in the production of bulk chemicals from renewable feedstocks. In addition, another characteristic of chemicals based on renewable feedstocks is that many alternative technologies and possible routes exist, resulting in many possible process flowsheets. The challenge for process engineers is then to choose between possible process routes and alternative technologies as well as to match different catalyst conditions. These kinds of problems are crucial, especially at the early stages of process development, when information is limited.

This thesis describes a methodological framework for dealing with the challenges and giving direction to research in the process development of chemicals based on renewable feedstocks. As an example, this thesis especially focuses on applying the methodology in process design and evaluation of the synthesis of 5-hydroxymethylfurfural (HMF) from the renewable feedstock glucose/fructose. The selected example is part of the chemoenzymatic process design of the synthesis 2,5-furandicarboxylic acid (FDA) from glucose.

By using the selected case study, the complexity and challenges for the process engineer to choose between different alternative routes and technologies as well as to combine two different kinds of catalysis (enzymatic catalysis and chemical catalysis) were illustrated.

Different process routes for the synthesis of HMF from fructose in the literature have been analyzed and evaluated. Using an aqueous route for HMF production is not economically feasible due to the low reaction yield. Using an anhydrous solvent for HMF synthesis is associated with high energy consumption and difficulties with solvent recycle in a large-scale production. The synthesis of HMF from fructose using a biphasic route is found to be promising, cost effective and give a better chance to be integrated with chemo-enzymatic cascades for producing FDA from glucose.

A process flowsheet using chemo-enzymatic cascades for HMF production from glucose has been proposed and evaluated. The process flowsheet is characterized by using glucose isomerase (EC 5.3.1.5) to convert glucose into fructose with a biphasic reaction for dehydration of fructose into HMF with recycle of the aqueous phase back to the enzymatic reaction. Costing analysis indicates the HMF production cost by the designed process is very sensitive to the dehydration reaction yield, the amount of solvent used in the whole process and the glucose price. In addition, increasing scale is also help to decrease the HMF production cost.

Using an ionic liquid (IL) route for HMF production has been evaluated with the dehydration reaction in [BMIm]Cl with different options starting from fructose and glucose with different initial concentrations. The HMF production cost is highly affected by the recycle of IL and catalyst. Processes with a high feed concentration show better economic potential than processes with a low feed concentration. IL processes starting from fructose are more costly than IL processes starting from glucose. A high concentration feed of glucose showed the best economic potential.

To sum up, the dehydration reaction yield is found to be the key important factor to achieve a feasible production cost of HMF. The use of the organic solvent can not be avoided and plays a very important role in determining the process economics. Recycling (unconverted sugar, reaction medium and solvent) become essential issues for HMF processes to reach a feasible production cost. Future directions and suggestions for the synthesis of HMF from sugar in a large-scale have been proposed. The developed methodology is helpful in evaluation and giving research directions. The methodology can be applied to other chemical process design and evaluation problems and in particular those for the next generation of production processes.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
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Biocatalysis is gaining ground in the pharmaceutical and fine chemical industry as a selective and potentially green technology to help synthesize industrially interesting products. In particular in the last decade the application of transaminases (E.C. 2.6.1.X) has gained particular attention as a means to synthesize optically pure chiral amines from prochiral ketones using an amine donor. Chiral amines can also be synthesized by other routes but the importance of the compounds mean that a variety of routes will be required to cover the synthesis of many different chiral amines of different properties and values.

A major challenge in the transaminase catalysed synthesis of chiral amines is the unfavourable equilibrium position [1]. There are several solutions to such equilibrium problems, including the use of in-situ product removal (ISPR) and cascade reactions to degrade or recycle the co-product formed. Such techniques, especially those using cascades can be a great tool to overcome the thermodynamic hurdle, but also present some new challenges with respect to compatibility of reaction conditions, recycling of co-factors and last but not least, the added cost of the cascade system components [2]. In this lecture we will present several process engineering tools including the use of mathematical modelling, uncertainty and sensitivity analysis [3] as well as economic evaluation and defined experimental protocols to help evaluate the feasibility of new biocatalytic cascades. The concepts will be illustrated with data from transaminase catalysed syntheses we have been modelling and studying experimentally at DTU.
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Main Research Area: Technical/natural sciences

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Process Intensification of the Production of Di-Methyl Carbonate (DMC) Using a New Synthesis and Design Process Intensification Methodology Framework

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Technical University of Dortmund
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Process/reactor selection for multistep biocatalysis.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Center for BioProcess Engineering
Authors: Xue, R. (Intern), Mikkelsen, J. D. (Intern), Meyer, A. S. (Intern), Woodley, J. (Intern)
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Process Synthesis, Design and Intensification: An Integrated Approach

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Carnegie Mellon University, Federal University of Uberlândia
Authors: Babi, D. K. (Intern), Woodley, J. (Intern), Gani, R. (Intern), Sirola, J. J. (Ekstern), Rodrigues, F. (Ekstern)
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Process Systems Engineering, 1. Introduction

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
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Process Technology for Immobilized Lipase-catalyzed Reactions

Biocatalysis has attracted significant attention recently, mainly due to its high selectivity and potential benefits for sustainability. Applications can be found in biorefineries, turning biomass into energy and chemicals, and also for products in the food and pharmaceutical industries. However, most applications remain in the production of high-value fine chemicals, primarily because of the expense of introducing new technology. In particular lipase-catalyzed synthesis has already achieved efficient operations for high-value products and more interesting now is to establish opportunities for low-value products. In order to guide the industrial implementation of immobilized-lipase catalyzed reactions, especially for high-volume low-value products, a methodological framework for dealing with the technical and scientific challenges and establishing an efficient process via targeted scale-down experimental work is described in this thesis. The methodology uses economic targets to test options characterized via a set of tools.

In order to validate the methodology, two processes based on immobilized lipase-catalysis have been studied: transesterification and esterification of vegetable oils for the production of biodiesel. The two processes are focused on the conversion of the two main components of vegetable oil materials, glyceride esters and free fatty acids respectively, into fatty acid alkyl esters. Although biodiesel is conventionally prepared via chemical-catalyzed transesterification of vegetable oils with methanol to produce fatty acid methyl esters (FAME), this work has been focused on the production of fatty acid ethyl esters (FAEE) with bioethanol due to the expected improved sustainability of this type of biodiesel. A key reaction characteristic of the immobilized lipase-catalyzed transesterification is that it is multi-phasic system. The by-product glycerol can potentially impose inhibitory effects on immobilized lipases and likewise the un-dissolved ethanol can inhibit the lipase. The options for addressing these issues can be used as the basis for selecting the biocatalyst and the reactor (e.g. a hydrophobic carrier for the immobilized lipase and the capabilities to provide sufficient mixing as well as stepwise/continuous feeding of ethanol to the reactor).

An STR is efficient for batch operation while a PBR is efficient for a continuous production. An STR can more easily provide sufficient external mass transfer for a reaction, but will lead to more mechanical damage of the biocatalyst particles, than a PBR. A reactor combination of CSTR with PBR can couple the advantages of both, delivering an efficient continuous process.

The second case study (esterification) shares some similar process characteristics to the first case (e.g. the multi-phasic nature). However, instead of glycerol, water shows a great impact on the extent of reaction. The removal of water should therefore be feasible during the operation of the reactor, either intermittently or preferably in situ. Highly anhydrous reaction conditions and the smaller substrates for this reaction place particular requirements on the lipase.

In order to validate the established processes at a larger scale, both lipase-catalyzed transesterification and esterification developed in the lab-scale STRs have been carried out in pilot-scale STRs. Results in both scale STRs correlate well with respect to the biocatalyst performance and mechanical stability.

Once the technical and scientific challenges of the process have been addressed, it is of course important to evaluate its economic and environmental feasibility. To that end, process evaluation has been performed for six processes composed of transesterification and product purification for making ‘in-spec’ biodiesel and the conventional chemical process is taken as a bench mark for comparison. The optimal process is a process composed of lipase-catalyzed transesterification with ‘in-spec’ biodiesel product as output with less feedstock input and waste production and much saved energy from the absence of product purification.
Process technology for multi-enzymatic reaction systems

In recent years, biocatalysis has started to provide an important green tool in synthetic organic chemistry. Currently, the idea of using multi-enzymatic systems for industrial production of chemical compounds becomes increasingly attractive. Recent examples demonstrate the potential of enzymatic synthesis and fermentation as an alternative to chemical-catalysis for the production of pharmaceuticals and fine chemicals. In particular, the use of multiple enzymes is of special interest. However, many challenges remain in the scale-up of a multi-enzymatic system. This review summarizes and discusses the technology options and strategies that are available for the development of multi-enzymatic processes. Some engineering tools, including kinetic models and operating windows, for developing and evaluating such processes are also introduced.
Production of Dialkyl Carbonates Via Reactive-Extractive and Pressure-Swing Distillations Using Unifac-CI VLE Model Predictions

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, ChemProcess Technologies
Authors: Dada, E. A. (Ekstern), Mustaffa, A. A. (Intern), Gani, R. (Intern)
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Production of ethanol from excess ethylene

Ethyl alcohol is one of the most important and used chemicals. Two common routes exist for the production: synthetic route typically based on petroleum feedstock and a fermentation route. The fermentation route comprises the majority of the produced ethyl alcohol. In this work, however, we will focus on the synthetic method, which employs direct hydration of ethylene. A conceptual process design of an ethyl alcohol producing plant is performed in a MSc-level course on Process Design at the Department of Chemical and Biochemical Engineering at DTU. In the designed process, 190 proof ethyl alcohol (azeotropic mixture) is produced from excess ethylene containing propylene and methane as impurities. The design work is based on a systematic approach consisting of 12 tasks performed in a specified hierarchy. According to this 12-tasks design procedure, information about the product and process is obtained in tasks 1-2. A preliminary process flowchart is obtained in task 3 using a modified Douglas hierarchical process synthesis method. The next tasks involves making design decisions and then further refining them in tasks 4-7 related to separation factors, reactor operating conditions, product purity, etc. In tasks 4 mass balances is are performed while in tasks 6-7 energy balances are performed. All simulations are made with PRO/II. Tasks 8-9 make the sizing and economic evaluation calculations. At this point, the base case design is obtained, which is then further refined and improved with respect to heat integration and process optimization (tasks 10-11). In the final task-12, the environmental impact of the process design is evaluated together with some of the key sustainability measures. In addition to PRO/II, the following software is used: ICAS (for property prediction, analysis) and ECON (cost and economic analysis). This design therefore covers all stages of conceptual design, starting from the consideration of qualitative aspects of the process flowsheet and preliminary calculations to detailed process simulations, equipment sizing, costing and an economic evaluation of the designed process. The resulting design utilizes 75 million kg/year ethylene feed in order to obtain an ethyl alcohol production of 90.5 million kg/year. The total capital investment has been estimated to 43 million USD and the total product cost without depreciation estimated to 58.5 million USD. Furthermore, computer aided economic analysis method has been applied to investigate the potential economic improvements. This analysis helps to define targets for improvement, which are then achieved through heat and mass integration as well as mathematical optimization. In the final step, the environmental impact of the process is analyzed and key sustainability factors such as energy used per kg of product, water used per kg of product, etc., are also determined. A sizable reduction of the operating costs has been possible through heat integration and process optimization yielding a 20 % reduction in total capital investment and a 15 % reduction in product cost without depreciation.

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Publication date: 2012

Property Modelling and Databases in Product-Process Design
Properties of pure chemicals and their mixtures play an important role in the design of chemicals based products and the processes that manufacture them. Although, the use of experimental data in the design and/or analysis of these chemicals based products and their processes is desirable, they are not always available. Also, it may be too expensive or it may take too long to measure the required data. In these situations and when repetitive calculations are involved, as in process simulation, it is useful to have appropriate models to reliably predict the needed properties. For property model development, however, it is necessary to have a large database of measured property data that has been checked for consistency and accuracy.

The presentation will first introduce a database, in terms of its knowledge representation structure, the type and range of properties and chemical systems covered, and their internal consistency-accuracy checks. The database includes properties of organic chemicals, polymers and ionic liquids. There are also chemical class specific database sections, such as for solvents, aroma-chemicals, surfactants and emulsifiers. The use of this property database for model development will then be highlighted for a class of predictive models employing the group-contribution approach, where, the group-contribution (GC) method is combined with the atom-connectivity index (CI) method. Here, two parallel models are developed using the same dataset. However, during applications for property prediction, only the GC-model is used with the option to estimate missing group-contribution parameters through the CI-model. In this way, the application range of the GC-model is increased without the need for additional experimental data. This procedure for model development and use has been successfully employed for a range of pure component properties, polymer repeat-unit properties as well as mixture properties. For the mixture properties, liquid phase activity coefficients are modelled and then
predicted through the UNIFAC-CI method. For bulk-properties of organic chemical mixtures, a GC-CI version of the PC-SAFT is used. The developed database and property prediction models have been combined into a properties-software that allows different product-process design related applications. The presentation will also briefly highlight applications of the software for virtual product-process design applications.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center  
Authors: Gani, R. (Intern), Sansonetti, S. (Intern)  
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Main Research Area: Technical/natural sciences

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**Property Prediction for Emulsion based Chemical Product Design**

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering  
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)  
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**Protein Dynamics in Organic Media at Varying Water Activity Studied by Molecular Dynamics Simulation**

In nonaqueous enzymology, control of enzyme hydration is commonly approached by fixing the thermodynamic water activity of the medium. In this work, we present a strategy for evaluating the water activity in molecular dynamics simulations of proteins in water/organic solvent mixtures. The method relies on determining the water content of the bulk phase and uses a combination of Kirkwood–Buff theory and free energy calculations to determine corresponding activity coefficients. We apply the method in a molecular dynamics study of Candida antarctica lipase B in pure water and the organic solvents methanol, tert-butyl alcohol, methyl tert-butyl ether, and hexane, each mixture at five different water activities. It is shown that similar water activity yields similar enzyme hydration in the different solvents. However, both solvent and water activity are shown to have profound effects on enzyme structure and flexibility.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Chemistry, Physical and Biophysical Chemistry
Biocatalysis (the use of one or more isolated enzymes in soluble or immobilized form, as well as enzymes contained within resting whole-cells) is a rapidly growing area of process technology. The introduction of biocatalysis presents new opportunities to develop ‘green’ synthetic routes to pharmaceuticals and other chemical products, since enzymes usually work in an aqueous solution and under mild conditions. Nevertheless the implementation of a biocatalytic reaction and the integration of a biocatalytic reaction into an otherwise chemical catalytic sequence is a complex task where PSE tools have a particularly important role to play. In this paper we will present a variety of PSE tools including computational fluid dynamics (CFD), operating windows, kinetic modelling, economic analysis and environmental assessment to support the development of economically viable biocatalytic processes.

Quantifying uncertainties of nucleation and crystal growth models on PAT system performance for crystallization processes

Quantifying uncertainties of nucleation and crystal growth models on PAT system performance for crystallization processes
Recent trends in modelling and simulation of biological nutrient removal systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Environmental Engineering, Environmental Chemistry, Center for Process Engineering and Technology, Lund University, Universidad Autonoma de Barcelona
Publication date: 2012
Main Research Area: Technical/natural sciences
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Recent trends in modelling and simulation of nutrient removal systems

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Main Research Area: Technical/natural sciences
Wastewater treatment, Modelling, Nutrient removal, Benchmark simulation
Source: dtu
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Reduction of a Mechanistic Drying Model of Pharmaceutical Granules for Inclusion in a Population Balance Model with Continuous Growth Term

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Ghent University
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Main Research Area: Technical/natural sciences
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AIChE_Paper 45a.pdf
Links:
https://aiche.confex.com/aiche/2012/webprogram/Paper260285.html

Relative importance of secondary settling tank models in WWTP simulations: A global sensitivity analysis using BSM2
Results obtained in a study using the Benchmark Simulation Model No. 1 (BSM1) show that a one-dimensional secondary settling tank (1-D SST) model structure and its parameters are among the most significant sources of uncertainty in wastewater treatment plant (WWTP) simulations [Ramin et al., 2011]. The sensitivity results consistently indicate that the prediction of sludge production is most sensitive to the variation of the settling parameters. In the present study, we use the Benchmark Simulation Model No. 2 (BSM2), a plant-wide benchmark, that combines the Activated Sludge Model No. 1 (ASM1) with the Anaerobic Digestion Model No. 1 (ADM1). We use BSM2 as a vehicle to compare two different 1-D SST models, and to assess the relative significance of their performance on WWTP simulation model outputs. The two 1-D SST models assessed include the first-order model by Takács et al. [1991] and the second-order convection-dispersion tool [Plósz et al., 2007]. Additionally, we assess the impact of two operational strategies for excess activated sludge wastage on simulation performance. A global sensitivity analysis (GSA) on BSM2 was carried out using two methods: (a) linear regression of Monte Carlo simulations (SRC method); and (b) Morris screening. The overall objective of assessing the 1-D SST model selection and parameters in GSA is to provide a parameter sensitivity ranking for WWTP calibration exercises, aiming at predicting key plant performance criteria, including methane production and effluent water quality index. Results obtained in this study show that, 1-D SST model parameters strongly influence biogas production via anaerobic digestion and the plant’s effluent water quality, but they have limited effect on estimating the quality of nitrogen rich returns from the digester.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Lund University
Authors: Ramin, E. (Intern), Flores-Alsina, X. (Ekstern), Sin, G. (Intern), Gernaey, K. (Intern), Jeppsson, U. (Ekstern), Mikkelsen, P. S. (Intern), Plósz, B. (Intern)
Number of pages: 8
Publication date: 2012

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Title of host publication: 2012 International Congress on Environmental Modelling and Software
Publisher: International Environmental Modelling and Software Society, iEMSs
Main Research Area: Technical/natural sciences
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Source: dtu
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Self-optimising control of sewer systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center, Technical University of Denmark
Authors: Castro, I. M. (Ekstern), Mauricio Iglesias, M. (Intern), Mollerup, A. L. (Intern), Sin, G. (Intern)
Publication date: 2012

Publications

Sensitivity analysis of autotrophic N removal by a granule based bioreactor: Influence of mass transfer versus microbial kinetics
A comprehensive and global sensitivity analysis was conducted under a range of operating conditions. The relative importance of mass transfer resistance versus kinetic parameters was studied and found to depend on the operating regime as follows: Operating under the optimal loading ratio of 1.90 (gO₂/m³/d)/(gN/m³/d), the system was influenced by mass transfer (10% impact on nitrogen removal) and performance was limited by AOB activity (75% impact on nitrogen removal), while operating above, AnAOB activity was limiting (68% impact on nitrogen removal). The negative effect of oxygen mass transfer had an impact of 15% on nitrogen removal. Summarizing such quantitative analyses led to formulation of an optimal operation window, which serves a valuable tool for diagnosis of performance problems and identification of optimal solutions in nitritation/anammox applications.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Department of Environmental Engineering, Environmental Chemistry
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Pages: 230-241
Publication date: 2012
Main Research Area: Technical/natural sciences
Sensitivity of Process Design due to Uncertainties in Property Estimates

The objective of this paper is to present a systematic methodology for performing analysis of sensitivity of process design due to uncertainties in property estimates. The methodology provides the following results: a) list of properties with critical importance on design; b) acceptable levels of accuracy for different thermo-physical property prediction models; and c) design variables versus properties relationships. The application of the methodology is illustrated through a case study of an extractive distillation process and sensitivity analysis of designs of various unit operations found in chemical processes. Among others vapour pressure accuracy for azeotropic mixtures is critical and needs to be measured or estimated with a ±0.25% accuracy to satisfy acceptable safety levels in design.
Sensitivity of process design to uncertainties in property estimates applied to extractive distillation

During the design of a chemical process, engineers typically switch from simple (shortcut) calculations to more detailed rigorous models to perform mass and energy balances around unit operations and to design process equipment involved in that process. The choice of the most appropriate thermodynamic and thermo-physical models is critical to obtain a feasible and operable process design and many guidelines pertaining to this can be found in the literature. But even if appropriate models have been chosen, the user needs to keep in mind that these models contain uncertainties which may propagate through the calculation steps to such an extent that the final design might not be feasible or lead to poor performance. Therefore, it is necessary to evaluate the sensitivity of process design to the uncertainties in property estimates obtained from thermo-physical property models. Uncertainty and sensitivity analysis can be combined to determine which properties are of critical importance from a process design point of view and to establish an acceptable level of accuracy for different thermo-physical property methods employed. This helps the user to determine if additional property measurements in the laboratory are required or to find more accurate values in the literature. A tailor-made and more efficient experimentation schedule is the result. This work discusses a systematic methodology for performing analysis of sensitivity of process design to uncertainties in property estimates. The application of the methodology is illustrated using a case study of extractive distillation in which acetone is separated from methanol using water as a solvent. Among others, the vapour pressure of acetone and water was found to be the most critical and even small uncertainties from -0.25% to +0.75% in vapour pressure data have shown a significant impact on the reflux ratio of the extractive distillation process.

In general, systematic sensitivity analysis should be part of process design efforts and expected to contribute to better-informed and reliable design solutions in chemical industries.
Simultaneous design of ionic liquid entrainers and energy efficient azeotropic separation processes

A methodology and tool set for the simultaneous design of ionic liquid entrainers and azeotropic separation processes is presented. By adjusting the cation, anion, and alkyl chain length on the cation, the properties of the ionic liquid can be adjusted to design an entrainer for a given azeotropic mixture. Several group contribution property models available in literature have been used along with a newly developed group contribution solubility parameter model and UNIFAC model for ionic liquids (UNIFAC-IL). For a given azeotropic mixture, an ionic liquid is designed using a computer-aided molecular design (CAMD) method and the UNIFAC-IL model is used to screen design candidates based on minimum ionic liquid concentration needed to break the azeotrope. Once the ionic liquid has been designed, the extractive distillation column for the azeotropic mixture is designed using the driving force method with a new proposed feed stage scaling to minimize energy inputs. Along with the distillation column, an ionic liquid recovery stage is designed and simulations are used to determine the overall heat duty for the entire process for the best ionic liquid candidates. Use of a designed ionic liquid reduces material and energy requirements when compared to an ionic liquid known to experimentally break a given azeotrope but not designed using CAMD methods. The acetone–methanol and ethanol–water azeotropes are provided as examples.
Simultaneous Design of Ionic Liquids and CO2 Recovery Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, University of Kansas
Authors: Chen, Q. (Ekstern), Christian, B. (Ekstern), Roughton, B. C. (Ekstern), Mitrofanov, I. (Intern), Camarda, K. C. (Ekstern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
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Links:
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Soft sensors in bioprocessing: A status report and recommendations

The following report with recommendations is the result of an expert panel meeting on soft sensor applications in bioprocess engineering that was organized by the Measurement, Monitoring, Modelling and Control (M3C) Working Group of the European Federation of Biotechnology - Section of Biochemical Engineering Science (ESBES). The aim of the panel was to provide an update on the present status of the subject and to identify critical needs and issues for the furthering of the successful development of soft sensor methods in bioprocess engineering research and for industrial applications, in particular with focus on biopharmaceutical applications. It concludes with a set of recommendations, which highlight current prospects for the extended use of soft sensors and those areas requiring development.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Hamburg University of Applied Sciences, University College London, Newcastle University, University of Applied Sciences Bremen, Richter-Helm GmbH, Siemens, University of Natural Resources and Life Sciences, Linköping University
Authors: Luttmann, R. (Ekstern), Bracewell, D. G. (Ekstern), Cornelissen, G. (Ekstern), Gernaey, K. (Intern), Glassey, J. (Ekstern), Hass, V. C. (Ekstern), Kaiser, C. (Ekstern), Preusse, C. (Ekstern), Striedner, G. (Ekstern), Mandenius, C. (Ekstern)
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Scopus rating (2012): SJR 0.944 SNIP 0.957 CiteScore 2.4
ISI indexed (2012): ISI indexed no
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Solventpro: The Solvent Selection and Design Framework

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mitrofanov, I. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
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State Estimation for the Automotive SCR Process

Selective catalytic reduction (SCR) of NOx is a widely applied diesel engine exhaust gas aftertreatment technology. For advanced SCR process control, like model predictive control, full state information of the process is required. The ammonia coverage ratio inside the catalyst is difficult to measure. Therefore we design an ordinary Kalman filter as well as an extended Kalman filter to estimate the ammonia coverage. The filters are built over a first principle model with four states. Among the four states, NO, NO2 and NH3 concentration are measured by the sensors, while the ammonia coverage ratio is left to be unknown. The performance of the filters is shown by simulation with the World Harmonized transient cycle. In particular, during transient operations the extended Kalman filter performs significantly better than the ordinary Kalman filter. Since such operation regimes are always present for SCR in engine applications, we recommend to estimating the ammonia coverage using the extended Kalman filter.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Zhou, G. (Ekstern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
Pages: 204
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Editors: Jørgensen, J. B., Huusom, J. K., Sin, G.
ISBN (Print): 978-87-643-0946-1
State Estimation in the Automotive SCR DeNOx Process

Selective catalytic reduction (SCR) of nitrogen oxides (NOx) is a widely applied diesel engine exhaust gas after-treatment technology. For effective NOx removal in a transient operating automotive application, controlled dosing of urea can be used to meet the increasingly restrictive legislations on exhaust gas emissions. For advanced control, e.g. Model Predictive Control (MPC), of the SCR process, accurate state estimates are needed. We investigate the performance of the ordinary and the extended Kalman filters based on a simple first principle system model. The performance is tested through a series of simulation studies reflecting realistic challenges such as under-modelling and few gas composition sensors.

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Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre, Haldor Topsoe AS
Authors: Zhou, G. (Intern), Jørgensen, J. B. (Intern), Duwig, C. (Ekstern), Huusom, J. K. (Intern)
Pages: 501-506
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State Estimation, Kalman Filtering, Nonlinear processes, SCR process
DOIs: 10.3182/20120710-4-SG-2026.00133
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

State-of-the-art and progress in the optimization-based simultaneous design and control for chemical processes

Significant progress in the area of simultaneous design and control for chemical processes has been achieved and various methodologies have been put forward to address this issue over the last several decades. These methods can be classified in two categories (1) controllability indicator-based frameworks that are capable of screening alternative designs,
and (2) optimization-based frameworks that integrate the process design and control system design. The major objective is to give an up-to-date review of the state-of-the-art and progress in the challenging area of optimization-based simultaneous design and control. First, motivations and significances of simultaneous design and control are illustrated. Second, a general classification of existing methodologies of optimization-based simultaneous design and control is outlined. Subsequently, the mathematical formulations and relevant theoretical solution algorithms, their merits, strengths and shortcomings are highlighted. Last, based on the recent advances in this field, challenges and future research directions are discussed briefly. An attempt is made with the help of this review article to stimulate further research and disseminate the simultaneous design methods to challenging problem areas. In particular, the application of optimization-based simultaneous design and control methods to large-scale systems with highly inherent nonlinear dynamics often the case in industrial chemical processes remains a challenging task and yet to be solved. © 2012 American Institute of Chemical Engineers AIChE J, 58: 1640–1659, 2012
Statistical modelling of the interplay between solute shape and rejection in porous membranes

The structural conformation of complex molecules, e.g., polymers and proteins, is determined by several factors like composition of the basic structural units, charge, and properties of the surrounding solvent. In absence of any chemical or physical interaction solute–solute and/or solute–membrane, it can be expected that the possibility for a solute particle to enter the membrane pore will only depend upon the relation between such molecular conformation and pore size. The objective of the present study is to use geometric and statistical modelling to determine the effect of particle elongation – from spherical to being increasingly prolate ellipsoidal – on the possibility of entering the pore, and, in turn, on the macroscopic distribution coefficient, K, and overall retention during filtration. The model showed that the value of K was maximal when the longer of the radii in the prolate ellipsoid was approximately equal to the radius of the pores, in case the spherical size of the particle was smaller than the membrane pore. Furthermore, for spherical particles larger than the pore, such a maximum was found to occur after the smaller of the radii was smaller than the pore radius. Either for spherical particles bigger or smaller than the pore radius, K was monotonically decreasing towards zero as the particles became more elongated. When relating the values of K to the friction model, the maximal rejection coefficient was found to reach a characteristic minimum when changing shape. The results suggested that the retention during porous membrane filtration can be manipulated when working with solute particles prone to alter conformation via, e.g., adding proper functional groups to the molecule, or modifying charge density/distribution by varying pH.
Synthesis and Design of Processing Networks: Stochastic Formulation and Solution

In this contribution, we propose an integrated business and engineering framework for synthesis and design of processing networks under uncertainty. In our framework, an adapted formulation of the transhipment problem is integrated with a superstructure, leading to a Stochastic Mixed Integer Non Linear Program (sMINLP), which is solved.
to determine simultaneously the optimal strategic and tactical decisions with respect to the processing network, the material flows, raw material and product portfolio. The framework allows time-effective and robust formulation, solution and analysis of largescale synthesis problems in presence of uncertainty parameters, contributing to broaden the range of application of stochastic programming and optimization to real industrial problems. The framework is applied to an industrial case study based on soybean processing, to identify the optimal processing network under market and technical uncertainty.

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
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Series: Computer - Aided Chemical Engineering
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Conference: 22nd European Symposium on Computer Aided Process Engineering, London, United Kingdom, 17/06/2012 - 17/06/2012
Mixed Integer Non Linear Programming (MINLP), Integrated business and engineering decision making
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**Synthesis and Design of Processing Networks: Decision Making Under Uncertainty**

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**Synthesis and design of processing networks: decision making under uncertainty and sensitivity analysis**

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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Main Research Area: Technical/natural sciences
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Synthesis of Industrial Water Networks

Water is a valuable resource of great relevance for industrial activities. As water will become scarcer, optimization of its use is of key importance. The issue of water allocation and reuse through mathematical optimization has been addressed in various literature works [1, 2]. However, most of the water networks proposed comprise few contaminants and do not consider critical parameters for wastewater treatment equipment, such as limiting inlet concentrations, flow rates, and other specific design constraints. Thus, these networks are arguably not fit to manage the complexity of a real industrial case (in terms of number of contaminants, number of processing options, design constraints etc.).

In this work, a systematic framework for the formulation and solution of water networks problems is proposed, based on the modification of an earlier work [3]. The optimization problem is formulated as a Mixed Integer Non Linear Programming (MINLP), which is solved to identify the best wastewater treatment process among a set of predefined alternatives, according to selected optimum criteria. The optimum criteria may be minimum operating, capital, or total cost, freshwater consumption, treated water discharge and/or concentration of a selected contaminant. The final design can then be refined through a more detailed model with any appropriate process simulator.

The methodology employed is as follows. First, the sources of wastewater and treatment objectives need to be identified. A superstructure of available technologies is used in order to identify process alternatives. The superstructure is built dividing the treatment operation in tasks to remove the various pollutants and considering process units currently used in industry. Then, the objective function is chosen and the problem is formulated as a MINLP optimization problem, which is solved in GAMS.

In order to demonstrate and highlight the features of the tool, a case study dealing with refinery wastewater purification is presented. A superstructure containing technological alternatives for water purification is built, and the optimization problem is formulated and solved for different scenarios. With respect to the superstructures presented in literature, the one developed here accommodates a more detailed modeling of the water treatment units and a wider range of contaminants. This makes it flexible for various applications and can be used to provide guideline for the process design of the treatment of different types of wastewater sources. This approach constitutes a useful and flexible tool to design wastewater treatment systems for new plant or retrofit or expansion of existing plants. The tool also allows for the evaluation of the effect of different scenarios e.g. different optimum criteria, wastewater sources, environmental regulations on water discharge, contaminant loads on purified water to recycle etc.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
Authors: Pennati, A. (Ekstern), Quaglia, A. (Intern), Gani, R. (Intern)
A systematic development of constitutive models within a generic modelling framework has been developed for use in design, analysis and simulation of crystallization operations. The framework contains a tool for model identification connected with a generic crystalliser modelling tool-box, a tool for data handling and translation as well as model application features. Through this framework it is possible, for a wide range of crystallization processes, to generate the necessary problem-system specific models; to identify the parameters for constitutive models; and to handle or translate raw crystallization data. Application of the systematic framework is highlighted through a sucrose crystallization case study, for which the parameters for nucleation and crystal growth are first estimated from the available measured data and are then applied to study the crystallization operation.

**General information**

*State:* Published  
*Organisations:* Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering  
*Authors:* Abdul Samad, N. A. F. B. (Intern), Meisler, K. T. (Intern), Gernaey, K. (Intern), von Solms, N. (Intern), Gani, R. (Intern)  
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**Systematic Multi-Scale Model Development Strategy for the Fragrance Spraying Process and Transport**

The fast and efficient development and application of reliable models with appropriate degree of detail to predict the behavior of fragrance aerosols are challenging problems of high interest to the related industries. A generic modeling template for the systematic derivation of specific fragrance aerosol models is proposed. The main benefits of the fragrance spraying template are the speed-up of the model development/derivation process, the increase in model quality, and the provision of structured domain knowledge where needed. The fragrance spraying template is integrated in a generic computer-aided modeling framework, which is structured based on workflows for different general modeling tasks. The benefits of the fragrance spraying template are highlighted by a case study related to the derivation of a fragrance aerosol model that is able to reflect measured dynamic droplet size distribution profiles for limonene.
Temperature Modelling of the Biomass Pretreatment Process

In a second generation biorefinery, the biomass pretreatment stage has an important contribution to the efficiency of the downstream processing units involved in biofuel production. Most of the pretreatment process occurs in a large pressurized thermal reactor that presents an irregular temperature distribution. Therefore, an accurate temperature model is critical for observing the biomass pretreatment. More than that, the biomass is also pushed with a constant horizontal speed along the reactor in order to ensure a continuous throughput. The goal of this paper is to derive a temperature model that captures the environmental temperature differences inside the reactor using distributed parameters. A Kalman filter is then added to account for any missing dynamics and the overall model is embedded into a temperature soft sensor. The operator of the plant will be able to observe the temperature in any point of the thermal reactor. Real data sets were extracted from the Inbicon biorefinery situated in Kalundborg, Denmark, and will be utilized to validate and test the temperature model.

General information

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Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, DONG Energy A/S
Authors: Prunescu, R. M. (Intern), Blanke, M. (Intern), Jensen, J. M. (Ekstern), Sin, G. (Intern)
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

ThermoData Engine: Extension to Solvent Design and Multi-component Process Stream Property Calculations with Uncertainty Analysis

ThermoData Engine (TDE, NIST Standard Reference Databases 103a and 103b) is the first product that implements the concept of Dynamic Data Evaluation in the fields of thermophysics and thermochemistry, which includes maintaining the comprehensive and up-to-date database of experimentally measured property values and expert system for data analysis and generation of recommended property values at the specified conditions along with uncertainties on demand. The most recent extension of TDE covers solvent design and multi-component process stream property calculations with uncertainty analysis.

Solvent Design function serves three tasks: (1) selection of best solvent for a solid solute, (2) search for a selective solvent for a solid binary mixture, and (3) selection of best solvent for extraction. Solvents are selected from the list of registered compounds encountering more than 27,000 entries. Selection is made by best efficiency (depending on the task, solubility, selectivity, or distribution coefficient, etc.) and matching other requirements requested by the user. At user's request, efficiency criteria are evaluated based on experimental data for binary mixtures or predictive models (UNIFAC variations). Predictions can be compared to the available experimental data, and uncertainties are estimated for all efficiency criteria. Calculations of the properties of multi-component streams including composition at phase equilibria (flash calculations) are at the heart of process simulation engines. However, the accuracy of such calculations are generally unknown that often leads to overdesign of the operational units and results in significant additional cost. TDE provides a tool for the analysis of uncertainty of property calculations for multi-component streams. A process stream in TDE can be either a pure substance or mixture of chemical compounds under bubble, dew, or specified P-T conditions. VLE compositions and single-phase
properties are calculated for process streams. Uncertainties are evaluated with the use of the covariance method where covariance matrices account for experimental uncertainties, curve deviations, and inadequacies of the models. Uncertainty analysis shows relative contributions to the total uncertainty from each component and pair of components.

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The Solvent Selection framework: solvents for organic synthesis, separation processes and ionic-liquids solvents

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mitrofanov, I. (Intern), Sansonetti, S. (Intern), Abildskov, J. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions: IGM_JA_GSI_RaG_ESCAPE22_abstract.pdf
Source: dtu
Source-ID: u::4400
Publication: Research › Conference abstract for conference – Annual report year: 2012

The Solvent Selection framework: solvents for organic synthesis, separation processes and ionic-organic synthesis

This paper presents a systematic integrated framework for solvent selection and solvent design. The framework is divided into several modules, which can tackle specific problems in various solvent-based applications. In particular, three modules corresponding to the following solvent selection problems are presented: 1) solvent selection and design for organic synthesis, 2) solvent screening and design of solvent mixtures for pharmaceutical applications and 3) ionic liquids selection and design as solvents. The application of the framework is highlighted successfully through case studies focusing on solvent replacement problem in organic synthesis and solvent mixture design for ibuprofen respectively.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mitrofanov, I. (Intern), Sansonetti, S. (Intern), Abildskov, J. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 762-766
Publication date: 2012

Host publication information
Title of host publication: Proceedings of the 22nd European Symposium on Computer Aided Process Engineering
Publisher: Elsevier Science
Series: Computer - Aided Chemical Engineering
Volume: 30
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 22nd European Symposium on Computer Aided Process Engineering, London, United Kingdom, 17/06/2012 - 17/06/2012
API, CAMD, Crystallization, Solvent selection framework, Solubility
Electronic versions: PEC12_08.pdf
Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

Tools for characterizing the whole-cell bio-oxidation of alkanes at microscale

This article describes the first reported microwell whole-cell bioconversion using a water immiscible substrate that matches the specific activity and yield achieved in a 1.2 L stirred tank bioreactor. Maximum yields of 0.6 g/Ltotal 1-dodecanol achieved in 24 h compare favorably to 0.28 g/Ltotal 1-dodecanol after 48 h obtained in a stirred tank reactor. Using the microwell platform we present a rapid and systematic approach to identify the key bottlenecks in the bio-oxidation of long-
chain alkanes using Escherichia coli expressing the alkane hydroxylase (alkB) complex. The results indicate that mass transfer rates limit productivity in the n-dodecane bio-oxidation system, rather than inherent enzyme activity. Furthermore, substrate solubility, oxygen availability and glucose concentration act cooperatively to affect the amount of by-product, dodecanoic acid. Optimizing these factors using response surface methodology enabled specific yields of 1-dodecanol to increase eightfold and overoxidation to dodecanoic acid to be reduced from 95% to 55%. This resulted in specific activities of 10.4 µmol/min/gdcw on n-dodecane; approximately 50% of the 21 µmol/min/gdcw obtained with n-octane. For the first time, this in vivo rate difference is within the range reported for the purified enzyme. Finally, the results obtained also provide strong evidence that the mechanism of E. coli interaction with alkanes is mainly via uptake of alkanes dissolved in the aqueous phase rather than by direct cell–droplet contact.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, University College London
Authors: Grant, C. (Ekstern), da Silva Damas Pinto, A. C. (Ekstern), Lui, H. (Ekstern), Woodley, J. M. (Intern), Baganz, F. (Ekstern)
Pages: 2179-2189
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Biotechnology and Bioengineering (Print)
Volume: 109
Issue number: 9
ISSN (Print): 0006-3592
Ratings:
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 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
Tools to evaluate processes for oxidase-based biocatalysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Ramesh, H. (Intern), Tufvesson, P. (Intern), Woodley, J. (Intern)
Number of pages: 21
Publication date: 2012

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Tools to evaluate processes for oxidase-based biocatalysis - Hemalata Ramesh.pdf

Bibliographical note
Oral presentation.
Source: dtu
Source-ID: u::5152
Publication: Research › Sound/Visual production (digital) – Annual report year: 2012

Topology Optimized Bioreactors — A Design Example with Immobilized Yeast

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Department of Systems Biology, Center for Microbial Biotechnology, Department of Micro- and Nanotechnology, Theoretical Microsystems Optimization
Authors: Lencastre Fernandes, R. (Intern), Schäpper, D. (Intern), Eliasson Lantz, A. (Intern), Okkels, F. (Intern), Bruus, H. (Intern), Gernaey, K. (Intern)
Number of pages: 30
Publication date: 2012

Publication information
Towards a plant-wide Benchmark Simulation Model with simultaneous nitrogen and phosphorus removal wastewater treatment processes.

It is more than 10 years since the publication of the Benchmark Simulation Model No 1 (BSM1) manual (Copp, 2002). The main objective of BSM1 was creating a platform for benchmarking carbon and nitrogen removal strategies in activated sludge systems. The initial platform evolved into BSM1_LT and BSM2, which allowed the evaluation of monitoring and plant-wide control strategies, respectively. The fact that the BSM platforms have resulted in 300+ publications demonstrates the interest for the tool within the scientific community. In this paper, an extension of the BSM2 is proposed. This extension aims at facilitating simultaneous carbon, nitrogen and phosphorus (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 phosphorus removal as an alternative to chemical P removal based on precipitation using metal salts, such as Fe or Al. This paper identifies and discusses important issues that need to be addressed to upgrade the BSM2 to BSM2-P, for example: 1) new influent wastewater characteristics; 2) new (bio) chemical processes to account for; 3) modifications of the original BSM2 physical plant layout; 4) new/upgraded generic mathematical models; 5) model integration; 6) new control handles/sensors; and 7) new extended evaluation criteria. The paper covers and analyzes all these aspects in detail, identifying the main bottlenecks that need to be addressed and finally discusses the aspects where scientific consensus is required.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Lund University, University of Queensland, University of KwaZulu-Natal, University of Cape Town
Number of pages: 8
Publication date: 2012
Main Research Area: Technical/natural sciences
Modelling, Benchmarking, Phosphorus removal, Model-based evaluation, Multi-criteria decision making, Process control
Electronic versions:
C_260_paper.pdf
Source: dtu
Source-ID: u::6266
Publication: Research - peer-review › Paper – Annual report year: 2012

Towards continuous enzyme-catalysed processes for the production of biodiesel

The application of lipases in the production of biodiesel can find several roles: in pretreating high FFA oils via esterification, transesterification for converting oil to biodiesel and polishing via esterification to ensure the product is within specification. In all these cases the potential size of the process plants, suggest that continuous operation would be highly beneficial due to the economies of scale. To investigate this, we have examined both oil pretreatment via esterification and biodiesel production via transesterification in batch stirred tank reactors (BSTRs), continuous stirred tank reactors (CSTRs) and continuous packed bed reactors (CPBRs). In addition comparisons have been made between the use of liquid enzyme (in CSTR and BSTR) and immobilized enzyme (in BSTR, CSTR and CPBR) in transesterification reactions. In this presentation an evaluation will be given of the alternative modes of operation based on experimental and modeled data from laboratory scale studies. Implications for scale-up will be discussed, together with guidelines for the implementation of continuous processes for enzymatic reactions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Authors: Nordblad, M. (Intern), Pedersen, A. K. (Intern), Meyland, L. H. (Intern), Xu, Y. (Intern), Woodley, J. (Intern)
Publication date: 2012
Event: Abstract from 103rd AOCS Annual Meeting & Expo, Long Beach, CA, United States.
Main Research Area: Technical/natural sciences
Links:
http://www.aocs.org/archives/am2012/index2.cfm?interest=Processing
Projects:

**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)

**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:

AI, Resul (Intern)

Ruszczynski, Lukasz (Intern)

da Conceicao Do Carmo Montes, Frederico (Intern)

Forero-Hernandez, Hector Alexander (Intern)

Jones, Mark Nicholas (Intern)

Supervisor:

Gernaey, Krist V. (Intern)

Abildskov, Jens (Intern)

Project Coordinator:

Sin, Gürkan (Intern)

**Engineered yeast strains for the production of bulk chemicals from algae biomass**
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.
Kærn, 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 Coordinator:
Sørensen, Iben (Intern)

Relations
Activities:
International Workshop on High Temperature Heat Pumps
Publications:
- Mapping of low temperature heat sources in Denmark
- Improving efficiency of heat pumps by use of zeotropic mixtures for different temperature glides
- Book of presentations of the International Workshop on High Temperature Heat Pumps
- Project report: Experimental planning and verification of working fluids (WP 5)
- Industrial Energy Mapping: THERMCYC WP6
- High Temperature Heat Pump Integration using Zeotropic Working Fluids for Spray Drying Facilities
- Forbedring af industrielle processers energieffektivitet
- Derivation of guidelines for the design of plate evaporators in heat pumps using zeotropic mixtures

Proyecto de 2ª Generación Biorefinaries Producción de 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:
Ógmundarson, 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
EasyClone 2.0
CRISPR–Cas system enables fast and simple genome editing of industrial Saccharomyces cerevisiae strains
Project

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
Project participant:
Krühne, Ulrich (Intern)
Bodla, Vijaya Krishna (Intern)
Gernaey, Krist V. (Intern)
Project

Activities:

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)
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/alive1, osmotically stressed2) and growth rate3. Furthermore, the cell size was recently correlated to the accumulation of an internal product (fatty acids) in microalgae4. 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 instrument5 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.

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
Bonita Springs, United States
Activity: Talks and presentations › Conference presentations

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
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**

**ECAB 4**  
01/10/2017 → 05/01/2018  
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
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)
Xavier Flores Alsina (Other)
Kasper Kjellberg (Other)
Jan-Michael Blum (Other)
Borja Valverde Pérez (Other)
Gürkan Sin (Other)
Barth F. Smets (Other)
Krist V. Gernaey (Other)
Department of Chemical and Biochemical Engineering
PROSYS - Process and Systems Engineering Centre
Department of Environmental Engineering
Degree of recognition: International

Related event

10th International Conference on Biofilm Reactors
09/05/2017 → 12/05/2017
Dublin, Ireland
Activity: Talks and presentations › Conference presentations

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
Degree of recognition: International

Related event

10th International Conference on Biofilm Reactors
09/05/2017 → 12/05/2017
Dublin, Ireland
Activity: Talks and presentations › Conference presentations

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

In-Silico Tailoring Properties of Poly(lactic acid)
Period: 13 Nov 2016 → 18 Nov 2016
Alexandr Zubov (Speaker)
Related event

2016 AIChE Annual Meeting
13/11/2016 → 19/11/2016
San Francisco, CA, United States
Activity: Talks and presentations › Conference presentations

EHEDG World Congress on Hygienic Engineering & Design 2016
Period: 2 Nov 2016 → 3 Nov 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

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

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

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

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

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

Related event

Advances in Process Analytics and Control Technology 2016
20/04/2016 → 22/04/2016
Chester, United Kingdom
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
24/11/2015 → 26/11/2015
Dresden, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

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

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

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
CAPEC-PROCESS

Related event
BioPro World Talent Campus 2015
17/08/2015 → 21/08/2015
Sore, Denmark
Activity: Talks and presentations › Conference presentations

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

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
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.

Multivariate analysis of industrial scale fermentation data
Lisa Mears (Speaker)
Department of Chemical and Biochemical Engineering

Gave an oral presentation at the ICOSSE 2015 Conference.

4th International Congress on Sustainability Science & Engineering
Period: 28 May 2015
Rebecca Frauzem (Speaker)
Department of Chemical and Biochemical Engineering

Correlated event

4th International Congress on Sustainability Science & Engineering
Period: 26/05/2015 → 29/05/2015
Balatonfüred, Hungary
Activity: Talks and presentations › Conference presentations
4th International Congress on Sustainability Science & Engineering
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

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

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
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

Microfluidics in Chemical and Biochemical Engineering Applications
Period: 23 Sep 2014
Ulrich Krühne (Lecturer)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS

Related event

8th Workshop "Low Flows in Medical Technology"
23/09/2014 → 24/12/2014
Lübeck, Germany

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

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

**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
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
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
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

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

**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

**Description**  
AstraZeneca, UK  
Selected external organisation

**Related external organisation**  
**Unknown external organisation**  
Activity: Talks and presentations › Conference presentations
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

Pesticide uptake modeling
Period: 7 Nov 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Rafiqul 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

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
Unknown external organisation
Activity: Talks and presentations › Conference presentations

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

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
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

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

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
Centre for oil and gas – DTU

Description
Poster presentation.

Related event

Biorefinery Öresund Conference 'Biorefining from raw material to high value products'
18/09/2013 → …
Ørestad, Denmark
Activity: Talks and presentations › Conference presentations

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

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

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

**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
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