Research outputs:

**Economic Risk Analysis and Critical Comparison of Biodiesel Production Systems**

In this chapter, the importance of risk assessment in biodiesel-based economy is first discussed. The importance of risk analysis to identify the most promising production schemes is also discussed from an economic point of view. Next, a systematic framework for economic risk assessment of biodiesel production processes and its associated by-products is presented. The application of the framework is highlighted through the production of 1,2-propanediol and 1,3-propanediol as value-added products from glycerol, which are 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. In order to decrease the economic risk, the integrated production of the product as a module added to the biodiesel plant was tested as an alternative scenario. Using the integrated concept of utilizing 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. The developed generic framework can be applied to other biodiesel by-products to assess the potentials of obtaining value-added products from them. Finally, future perspectives and other approaches toward economic production of biodiesel with lower risks are highlighted. The framework proposed in this work is to provide some detailed perspectives to facilitate the economic risk analysis of biodiesel production for any given technology.
A methodology for uncertainty analysis of reference equations of state

We present a detailed methodology for the uncertainty analysis of reference equations of state (EOS) based on Helmholtz energy. In recent years there has been an increased interest in uncertainties of property data and process models of thermal systems. In the literature there are various methodologies to assess uncertainty of measured property data. Currently there is still a lack of methodologies to quantify property uncertainties from property models, such as EOS. EOS developers and users either do not report uncertainties or report underestimated values. In this work linear approximation for uncertainty analysis is suggested as a tool for EOS. The uncertainties of the EOS properties are calculated from the experimental values and the EOS model structure through the parameter covariance matrix and subsequent linear error propagation. This allows reporting the uncertainty range (95% confidence interval) of every EOS property value. As an example the Helmholtz-based EOS of propane is thoroughly analysed with respect to its uncertainty. The results show, in which temperature and pressure ranges, high and low property uncertainties occur. The uncertainty methodology is generic and can be applied for any novel EOS. Furthermore, the methodology is suitable for already existing EOS, since re-training of the data is not necessary. The study clearly demonstrates that a thorough uncertainty analysis gives valuable insights for EOS users and developers.

General information
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Contributors: Cheung, H., Frutiger, J., Bell, I. H., Abildskov, J., Sin, G., Wang, S.
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A probabilistic model-based soft sensor to monitor lactic acid bacteria fermentations

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, PILOT PLANT, Chr. Hansen AS
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Pages: 49-60
A Water Treatment Case Study for Quantifying Model Performance with Multilevel Flow Modeling

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

General information
State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Centre for oil and gas – DTU, Aalborg University
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ISI indexed (2013): ISI indexed yes
Scopus rating (2012): CiteScore 0.86 SJR 0.808 SNIP 1.38
Web of Science (2012): Impact factor 0.576
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): CiteScore 0.73 SJR 0.475 SNIP 0.914
Web of Science (2011): Impact factor 0.487
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Computer-aided molecular product-process design under property uncertainties – A Monte Carlo based optimization strategy

A methodology is presented to solve a computer-aided molecular design (CAMD) and process design model problems under consideration of fluid property uncertainty. The uncertainties of the group contribution (GC) property prediction models are quantified for which asymptotic approximation of the covariance of parameter estimation errors is performed following a regression analysis. A Monte Carlo sampling technique generates GC factor samples within the respective uncertainties, which are evaluated separately as constraints to the CAMD optimization problem. The methodology is applied to identify working fluid candidates for an organic Rankine cycle used as waste heat recovery system in a marine diesel engine. CAMD under property uncertainties allows 1) identifying robust and more reliable molecules with respect to property uncertainties (conservative approach) and 2) enhancing the search space in order to find potentially globally optimal working fluids (optimistic approach). Suitable Hydrofluoroolefins (HFO) have been identified as potential working fluids for waste heat recovery.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
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Web of Science (2017): Impact factor 3.113
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BFI (2016): BFI-level 2
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Web of Science (2016): Impact factor 3.024
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BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.713
Web of Science (2015): Impact factor 2.581
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.22 SJR 1.168 SNIP 1.728
Web of Science (2014): Impact factor 2.784
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.06 SJR 1.21 SNIP 1.744
Web of Science (2013): Impact factor 2.452
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.05 SJR 1.136 SNIP 1.897
Web of Science (2012): Impact factor 2.091
Design and preliminary operation of a hybrid syngas/solar PV/battery power system for off-grid applications: A case study in Thailand

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

**General information**

State: Published
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.821 SNIP 1.348
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.7 SJR 0.852 SNIP 1.434
Web of Science (2015): Impact factor 2.525
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BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.91 SJR 1.022 SNIP 1.671
Web of Science (2014): Impact factor 2.348
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.56 SJR 0.953 SNIP 1.673
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.31 SJR 0.918 SNIP 1.611
Web of Science (2012): Impact factor 1.927
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.12 SJR 0.903 SNIP 1.327
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.87 SNIP 1.32
Web of Science (2010): Impact factor 1.519
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.741 SNIP 1.018
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Design, Global Sensitivity Analysis and Optimisation of a Counter-current Spray Column for Splitting Triglyceride Mixtures

We present the model of a counter-current spray column which hydrolyses mixtures of triglycerides with water and leads to fatty acids and glycerol. A finite volumes model was implemented in Fortran and validated with an analytical model derived from experimental data found in literature. Global, variance-based (Sobol) sensitivity analysis allowed to assess the sensitivity of the sweet water glycerol content to liquid density, overall mass transfer coefficient, reaction rate coefficient and the equilibrium ratio to rank them accordingly and to evaluate if the confidence intervals of the predicted properties are acceptable in respect to the calculated design or economic costs. Monte-Carlo based optimisation was performed to minimize operating cost varying the steam inlet flow rate and distribution as the independent variables. This model-based approach allows to be adapted to different spray column setups and gives the engineer a valuable tool to validate, analyse and optimise an industrial scalespray column. The possibility to perform parameter estimation is given if experimental data from an existing plant is provided.

Dynamic plantwide modeling, uncertainty and sensitivity analysis of a pharmaceutical upstream synthesis: Ibuprofen case study

A dynamic plantwide model was developed for the synthesis of the Active pharmaceutical Ingredient (API) ibuprofen, following the Hoescht synthesis process. The kinetic parameters, reagents, products and by-products of the different reactions were adapted from literature, and the different process operations integrated until the end process, crystallization and isolation of the ibuprofen crystals. The dynamic model simulations were validated against available measurements from literature and then used as enabling tool to analyze the robustness of design space. To this end, sensitivity of the design space towards input disturbances and process uncertainties (from physical and model parameters) is studied using Monte Carlo simulations. The results quantify the uncertainty of the quality of product attributes, with particular focus on
crystal size distribution and ibuprofen crystalized. The ranking of the most influential parameters on the chosen quality attributes is presented, with crystal growth and water concentration being the most influential ones. The total amount of saturated solvent, which propagates from upstream processes, has been shown to highly influence the total mass of crystal produced, and the target specifications for the API as well. This dynamic plantwide modeling coupled with Monte Carlo simulations is valuable to improve design and optimization of pharmaceutical processes at early stages, especially to bottleneck the design space against a range of uncertainties and disturbances.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre
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Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
Web of Science (2017): Impact factor 3.141
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.87 SJR 0.938 SNIP 1.145
Web of Science (2015): Impact factor 2.567
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.85 SJR 1.009 SNIP 1.287
Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.6 SJR 0.975 SNIP 1.232
Web of Science (2013): Impact factor 2.235
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.56 SJR 1.054 SNIP 1.32
Web of Science (2012): Impact factor 2.206
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.58 SJR 1.076 SNIP 1.236
Web of Science (2011): Impact factor 2.237
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.049 SNIP 1.161
From property uncertainties to process simulation uncertainties – Monte Carlo methods in SimSci PRO/II process simulator

This study presents a methodology to apply Monte Carlo methods for property uncertainty propagation in the process simulation software SimSci PRO/II. The aim of this work is to integrate advanced uncertainty and sensitivity analysis tools into commercial process simulators. The property uncertainty and sensitivity analysis tools were applied to a heat pump system with cyclopentane as a working fluid. Monte Carlo sampling technique was used to generate property samples of the SRK equation of state parameters critical temperature, critical pressure and acentric factor. The samples were subsequently evaluated in the heat pump flowsheet built in SimSci PRO/II. This allowed describing the process model output uncertainty in a distribution and with the 95% confidence interval. Furthermore, Monte Carlo based standard regression could be used to analyse the sensitivity of the respective fluid properties. The results showed that property uncertainty propagation strongly depends on the correlation between the property parameters. The sensitivity analysis showed that the acentric factor is the most sensitive SRK parameter. This work demonstrates that Monte Carlo methods are a simple and useful tool, which can be used in commercial process simulators by industrial users.

General information
State: Published
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Land-use planning risk estimates for a chemical industrial park in China - A longitudinal study

A chemical industrial park (CIP) can centralize the management of companies and facilitate mutual communication between different businesses. Due to these advantages, an increasing number of chemical companies are forced into CIP, especially in developing countries such as China. Thus, the land-use planning of CIP associated with safety becomes an important issue. To illustrate the importance of the continuous risk supervision and give more experiences to other similar changing CIP, we apply a simplified quantitative risk assessment procedure to estimate the risk to a Chinese chemical industrial park (19 x 10 km²) near a rather densely populated off-site region for the years 2014 and 2017. Estimated levels of individual risk and societal risk are compared with Chinese risk acceptance criteria for land-use planning. Off-site risk levels have increased significantly from 2014 to 2017. While off-site risk levels are still low and within the acceptable region, the study concludes that the authorities should review carefully and monitor the risk level in case of future development activities around and within the chemical industrial park, e.g. preserving a buffer zone should be considered. For future chemical park design, it is highly recommended to proactively include QRA analysis especially to deal with risk in an efficient way.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Statistics and Data Analysis, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, China University of Mining And Technology, COWI AS, China Academy of Safety Science and Technology
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.9 SJR 0.464 SNIP 0.8
Web of Science (2016): Impact factor 0.812
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.75 SJR 0.409 SNIP 0.73
Web of Science (2015): Impact factor 0.516
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.59 SJR 0.409 SNIP 0.91
Web of Science (2014): Impact factor 0.464
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.81 SJR 0.604 SNIP 2.027
Web of Science (2013): Impact factor 0.593
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BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.02 SJR 0.494 SNIP 1.603
Web of Science (2012): Impact factor 0.717
Model-based process development for a continuous lactic acid bacteria fermentation

A mechanistic process model describing a lactic acid bacteria (LAB) fermentation was applied to develop a continuous fermentation process. Producing LAB for the dairy industry in a continuous cultivation, which would allow harvesting the cells during the cultivation, would reduce production costs compared to traditional batch processes. To this end, a validated mechanistic model of a *Streptococcus thermophilus* fermentation was used for a model-based continuous process evaluation. The fermentation model consists of biological and chemical mechanisms including a description of the growth rate as a function of pH and inhibition effects of metabolites. The optimal dilution rate and substrate concentration in the feed were estimated in order to maximize the cell yield (biomass concentration) and to minimize the waste of substrate during the continuous fermentation in a 50 m³ bioreactor for two scenarios: downstream capabilities are i) flexible, and ii) fixed. The biomass concentration is restricted by the growth-inhibiting lactic acid concentration, which is produced by the growing bacteria. Furthermore, the substrate, which is supplied by the feed, should be consumed completely in the fermentation and not wasted in the bioreactor effluent owing to raw material costs. The resulting non-linear optimization problem was formulated and solved in MATLAB®. A Monte Carlo simulation showed the robustness of the results, where a biomass concentration of 5 g L⁻¹ could be achieved in the continuous fermentation with a substrate wastage of less than 3 % in the bioreactor effluent. The productivity of the continuous process was similar to a traditional batch process, but frequent cleaning and sterilization are no longer necessary in a continuous process resulting in a shorter unproductive downtime of the bioreactors. This promising potential of a continuous process for LAB cultivations encourages pilot-scale studies for a comprehensive techno-economic evaluation.

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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, PILOT PLANT, Chr. Hansen AS
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Modelling for Process Risk Assessment in Industrial Bioprocesses

The objective of this contribution is to give an overview about model implementations for risk-based decision making in industrial bioprocesses, such as the antibiotic production for the pharmaceutical industry. It focuses on the applications of mechanistic and computational fluid dynamics (CFD) models. The models are built to support the understanding of the process, improve or speed up the process development, and used to monitor and control the production process to achieve the desired product quality and quantity. Uncertainties inherently present in development of these models are considered in many applications, for example, by for example using Monte Carlo simulations, to enable a risk-based decision making when the model results from Monte Carlo simulations are assessed. The sources of uncertainties may include for example process input variations, model parameter uncertainty, assumptions underlying the model structure, and measurement errors, among others. More and more studies combine mechanistic biochemical models with CFD models to investigate especially heterogeneous process conditions at large scale such as substrate gradients. However, on-line applications of CFD models, for example, for process control, are hampered by the long computation times. Instead, CFD modeling efforts are directed towards supporting CFD-based compartment modeling that reduces the spatial resolution, but allows a much faster simulation compared to a CFD model. Compartment models integrating bio-kinetics of the bioprocess, various sources of uncertainties in the system, and heterogeneities in the bioreactor can then be applied as an enabling tool for risk-based on-line monitoring and control systems to achieve optimized bioprocess operations.

Modelling, Uncertainty and Sensitivity Analysis of the Batch Thermal Hydrolysis of Vegetable Oils

The oleochemical industry is of key relevance to food and cosmetic manufacturers as well as it represents a sustainable source of chemicals and liquid fuel. It is therefore of considerable interest to improve the understanding of design and operating variables that increase the feasibility of vegetable oil utilization. Modelling of batch systems is important for the industrial application of the fat/oil splitting process, because it provides information that could be used to compare different modelling approaches under different operating conditions for producing fatty acids.

In this paper, a rigorous kinetic and mass transfer model describing the batch hydrolysis of vegetable oil at subcritical conditions is presented. The developed model was further investigated using Monte Carlo simulations to statistically quantify the variability in the model outputs due to uncertainties in the parameter estimates. To understand which input parameters are responsible for the output uncertainty, a global sensitivity method (Morris screening) was used. The results from the sensitivity analysis helped to identify what parameters are influential to the model outputs, giving insight into how well the model predicts the concentrations of fatty acids and glycerol; which forms the basis for any model-based decision making for detailed process characterization, design, optimization and operation of the fat/oil splitting process.
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.
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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Trojan Technologies
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BFI (2018): BFI-level 1
This article presents a critical review on process synthesis, design, and control of wastewater treatment plants (WWTPs) which remains as an important task for researchers and design engineers working in the field. The motivations for and the challenges remaining in process synthesis, design, and control of WWTPs are firstly identified. The commonly used approaches for process synthesis, design, and control are then introduced with regards to their applicability to wastewater
treatment. To illustrate the frameworks for process synthesis, design, and control, two literature reported studies are used as examples. Applications of process synthesis, design, and control at WWTPs are summarized and discussed. To conclude the chapter, perspectives on process synthesis, design, and control of WWTPs are presented.

General information
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Research output: Research - peer-review | Book chapter – Annual report year: 2018

Property Prediction of Pharmaceuticals for Designing of Downstream Separation Processes
Downstream processing of pharmaceuticals is often a complex and expensive process section in pharmaceutical industry. The separation and purification cost of small to medium-sized active pharmaceutical ingredients (APIs) can be up to 70-90% of the total production cost. Designing a downstream processing includes selection, arrangement and rigorous evaluation of various unit operations such as crystallization and extraction. Solvent screening and selection is a critical step in designing such unit operations. The solubility of APIs is a major property for solvent screening and selection. Solubility can either be determined experimentally or by using predictive thermodynamic models. However, experimental solvent screening is most often expensive and laborious, or sometimes simply not possible due to the lack of sufficient amount of an API. Moreover, designing some unit operations; for example, crystallization further requires solubility property of an API as a function of temperature, solvent composition and pH for cooling, antisolvent and reactive crystallization, respectively, or any combination thereof.

In this work, different predictive thermodynamic models such as COSMO-SAC, COSMO-RS, NRTL-SAC and UNIFAC were applied for solubility prediction of a large molecular weight steroid-like structure antibiotic. The predicted solubility data were compared with experimental solubility data in a set of various solvents representative of wide solvent properties. Therefore, a model which gives more accurate solubility prediction can be selected. For this specific case study, the root mean square errors (RMSEs) of COSMO-SAC, UNIFAC, COSMO-RS and NRTL-SAC are 54.3%, 51.8%, 34.3% and 4.8%, respectively. NRTL-SAC was selected as a property prediction tool for solvent screening and selection as well as for further designing and optimization of crystallization unit operation. Moreover, global sensitivity and uncertainty analyses of the predictive thermodynamic model parameters were performed in order to identify sources of uncertainty and evaluate their influence.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Centre for oil and gas – DTU
Contributors: Molla, G. S., Ruszczynski, L., Abildskov, J., Sin, G.
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Reverse engineering of working fluid selection for industrial heat pump based on Monte Carlo sampling and uncertainty analysis

This study presents a novel methodology for the identification of suitable pure component working fluids for heat pumps. Two challenges are addressed: the difficulties in solving a complex product-process design problem and making it accessible for practical applications, as well as the impact of the working fluid property uncertainties on the solution. A Monte Carlo sampling is applied to generate sets of different property parameter combinations (virtual fluids), which are subsequently evaluated in the heat pump process model. The distance between the property values of the virtual fluid and the uncertainty bound of the properties of real fluids (collected from a database) are calculated. The fluids that are closest to the top-performing virtual fluids are further analyzed through evaluation in the cycle and subsequent uncertainty propagation of the respective input property uncertainties to the model output uncertainties. The methodology has been applied to an industrial heat pump system used for waste heat recovery from a spray drying facility in dairy industry. To remain focused on the validation of underlying concepts of the methodology, the study considered screening only among cyclic hydrocarbon working fluids. The compounds identified by the methodology had a low global warming potential.
Superstructure Optimisation with General Disjunctive Programming and Surrogate Models

In this work we present a framework to generate surrogates from rigorous process models embedded in a modelling environment or a process simulator. These unit operations (i.e. process flowsheet subsystems) are treated as black-box models to generate data for fitting and deriving surrogate functions. Further, the methodology includes the formulation of a superstructure optimisation problem in form of a general disjunctive program (GDP) and the identification of the optimal process flowsheet structure and point of operation from the possible alternatives. The superstructure optimisation incorporates selection and interconnection of each unit operation in form of disjunctions and with the objective to maximize profit or to minimize total cost. In this paper we highlight the surrogate building step of the methodology with a rigorous counter-current spray column model and a continuous stirred tank reactor (CSTR). We assess the performance of different surrogate modelling methods such as multivariate regression splines, polynomial chaos expansion and Gaussian process regression in respect to the coefficient of determination (R2), the mean squared error (MSE) and the learning curve performance. The GDP is either solved by transforming it to a MINLP via convex-hull and then solving the problem with a nonlinear solver or by applying directly the GDPopt solver which makes use of the logic based outer-approximation (OA) algorithm. We show that superstructure generation with surrogate models elevates rigorous process design to the upper layer of optimisation where the best sequence of unit operations is determined and raw material input streams, unit operation conditions and product purity are optimized simultaneously. Our proposed methodology and software tool helps
engineers to concentrate on the formulation and data retrieval tasks while trial and error simulations of different process configurations is prevented. A spreadsheet interface allows for easy data input and hides the underlying Fortran, Python and Pyomo scripts which can be accessed if the more sophisticated user wants to add new features to the framework.

**Superstructure Optimization of Oleochemical Processes with Surrogate Models**

In this work we present a framework to generate surrogate models from rigorous process models embedded in a modelling environment or a process simulator. These unit operations (i.e. process flowsheet subsystems) are treated as black-box models to generate data for fitting and deriving the surrogate. Further, the methodology includes the formulation of a superstructure optimization problem and solving it to identify the optimal process flowsheet structure and point of operation from the possible alternatives. The superstructure optimization incorporates selection and interconnection of each surrogate and multi-objective optimization in respect to total annual cost and environmental impact. In this paper we highlight the surrogate building step of the methodology with a rigorous counter-current spray column model and assess the performance of different surrogate modelling methods.

**Svovlsyres fortyndingsvarme**

[Dansk sammendrag] Det er god latin, at syrer fortyndes ved at hælde syren i vand, aldrig omvendt. Der udvikles betydelige mængder varme, og kogning kan slynge syre og vand ud af beholderen. Selvom svovlsyre anvendes i enorme mængder, er det overraskende vanskeligt at finde data for fortyndingsvarmen. Det rådes der bod på med denne artikel

[English summary] Although sulfuric acid is one of the most fundamentally important heavy industrial chemicals and produced in very large quantities, there is little practical guidance in open sources on how to estimate the heat of dilution. This article provides a simple method to estimate the increase in temperature upon diluting sulfuric acid with water. simple method to estimate the increase in temperature upon diluting sulfuric acid with water.
Uncertainty Analysis of the Experimental Results of Air Conditioner Performance due to Uncertainty of Equation of States

In previous literature, the uncertainty analyses of experimental results of air conditioners usually ignored the uncertainty due to the equation of state (EoS) of the refrigerants. One possible reason was that the uncertainty reported in the EoS literature was much smaller than the one of the measurement. However, with the advancement of the measurement technologies, the impact of measurement uncertainty on the air conditioner performance calculation is lowered and becomes on par with that of the EoS. Simultaneously, new research findings give more comprehensive understanding of the EoS uncertainties, such as that the uncertainty of EoS reported in previous studies was underestimated under some conditions. To examine if the uncertainty of experimental results of a thermal system are significantly affected by the new findings, an uncertainty analysis is carried out with experimental data of an air conditioner using propane. The results show that the uncertainty of EoS has a more significant impact on experimental results involving saturation temperature such as subcooling and superheat measurement than the uncertainties of the measurement, while its impact on the uncertainty of the measured heat transfer rate is still not as significant in most cases.

General information
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Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Hong Kong Polytechnic University, National Institute of Standards and Technology
Contributors: Cheung, H., Frutiger, J., Bell, I. H., Abildskov, J., Sin, G., Wang, S.
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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  
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**Article in proceedings – Annual report year:** 2017

**An Empirical Model for Carbon Recovery in a Rotating Belt Filter and Its Application in the Frame of Plantwide Evaluation**

The rotating belt filter (RBF) is an emerging and enabling technology for carbon recovery and also an alternative to the primary clarifier (PC), sludge thickening and dewatering. A recent study indicates that the RBF has the potential to reduce capital cost, footprint and improve energy and nutrient recovery in comparison to a conventional PC. Moreover, it is also believed that the RBF can fractionate carbon (enrichment of cellulose, namely toilet paper) based on particulate size, more efficiently than a PC. It is, therefore, necessary to understand and quantify the uniqueness of the RBF performance to maximize plant-wide benefits when retrofitted in existing wastewater treatment plants (WWTPs). Thus, a rigorous plant-wide study is required to interpret the deeper influence of an RBF on the major downstream units (such as activated sludge tanks, sludge digester, etc.). This study emphasizes the development of a simplified empirical model for describing carbon recovery in an RBF and the impact of the RBF implementation on plant-wide evaluation.

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**Organisations:** Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Trojan Technologies  
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**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 NH₄OH oxidation as the main N₂O producing pathway, a cascade controller configuration adapting the oxygen supply to respect only the effluent ammonium concentration limits was found to be more effective to ensure low N₂O emissions.
A novel model-based control strategy for aerobic filamentous fungal fed-batch fermentation processes

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

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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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Environmental Engineering, Novozymes AS
Contributors: Mears, L., Stocks, S. M., Albæk, M. O., Sin, G., Gernaey, K. V.
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Web of Science (2017): Impact factor 3.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.447 SNIP 1.178
Web of Science (2016): Impact factor 4.481
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.44 SJR 1.632 SNIP 1.355
Web of Science (2015): Indexed yes
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BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.44 SJR 1.637 SNIP 1.427
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.04 SJR 1.62 SNIP 1.364
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.08 SJR 1.668 SNIP 1.481
Web of Science (2011): Impact factor 3.946
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Scopus rating (2010): SJR 1.551 SNIP 1.354
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Scopus rating (2009): SJR 1.498 SNIP 1.358
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Scopus rating (2002): SJR 1.117 SNIP 1.263
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.059 SNIP 1.16
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A review of control strategies for manipulating the feed rate in fed-batch fermentation processes

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

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

**Biorefinery Sustainability Analysis**

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

**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.

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, Technical University of Denmark
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Web of Science (2016): Impact factor 6.942
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Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
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Calibration of the NDHA N2O model via respirometric assays

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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.

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Contributors: Frutiger, J., Cignitti, S., Abildskov, J., Woodley, J., Sin, G.
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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.

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Scopus rating (2016): CiteScore 1.87 SJR 0.769 SNIP 1.261
Control of N2O-emissions by aeration

Disclosed herein is a method and a system for controlling N2O emission from a water-based solution containing nitrifying organisms, wherein an input variable for a controller is the ratio between NO3 - produced and NH4 + oxidized as determined by measuring NO3 - and NH4 + concentration both at the inlet and at the outlet of the aerated section containing the water-based solution with nitrifying organisms and a scaled output variable is obtained from the controller as a function of said ratio by a non-linear algorithm, so that the oxygen input and/or the aeration time is varied based on an integration of the deviations of said output variable.

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IPC: C02F3/00; C02F3/02
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Data Validation and Modelling of Thermodynamic Properties of Systems with Active Pharmaceutical Ingredients (APIs) in Complex Media for Skin Absorption Processes

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

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Contributors: Ruszczynski, L., Zubov, A., Sin, G., Abildskov, J.
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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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Novozymes A/S, LEO Pharma AS
Contributors: Mears, L., Stocks, S. M., Albaek, M. O., Sin, G., Gernaey, K. V.
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BFI (2018): BFI-level 2
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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Maria Dragan, J., Zubov, A., Sin, G.
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Model-based plant-wide optimization of large-scale lignocellulosic bioethanol plants.

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

General information
State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, DONG Energy AS
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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, require rigorous and reliable model building and testing. Multilevel Flow Modeling is a qualitative method for diagnosing faults, and has previously only been validated by subjective and qualitative means. This work aims to synthesize a procedure to measure model performance, according to diagnostic requirements, to ensure reliability during operation. A simple procedure is proposed for validating and evaluating Multilevel Flow Modeling models. For this purpose expert statements, a dynamic process simulation in K-spice, and pilot plant experiments are used for validation of two simple Multilevel Flow Modeling models of a deoiling hydrocyclone, used for water and oil separation.

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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.

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N2O and NO dynamics in AOB-enriched and mixed-culture biomass: experimental observations and model calibration

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N2O and NO dynamics in AOB-enriched and mixed-culture biomass: Experimental Observations and Model Calibration

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

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Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203  
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Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155  
Web of Science (2016): Impact factor 2.843  
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BFI (2015): BFI-level 2  
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BFI (2011): BFI-level 2
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.
Superstructure-based optimization tool for plant design and retrofitting

Many wastewater treatment processes and technologies have been developed since the beginning of the 20th century to meet increasingly stringent performance demands. Still the wastewater industry has been facing many new challenges such as increasing energy costs, presence of trace organics which has become more critically investigated, depletion of the resources, water conservation as well as more stringent regulations (Reardon et al. 2013).

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).
Techno-economic analysis of resource recovery technologies for wastewater treatment plants

The high nutrient content of domestic wastewater can be efficiently recovered through specific technologies included in dedicated wastewater treatment plants (WWTPs). Nevertheless, the operational costs linked to the implementation of these technologies can make them economically unfeasible. It is therefore important to evaluate the best way to upgrade an already existing WWTP from an economic point of view. In the present work, this is virtually done by using a simulation model, namely the Benchmark Simulation Model no2 (BSM2), as base case study. The BSM2 is extended by including the following resource-recovery treatment units: (a) a chemical precipitation process, for recovery of iron phosphate fertilizer; (b) the Exelys technology, for increased biogas production; and, (c) the Phosnix technology, for recovery of struvite fertilizer. Seven upgrade strategies/flowsheets employing different combinations of the recovery technologies are generated and evaluated. The evaluation results have shown that the most economically beneficial strategy to upgrade the WWTP is to employ a Phosnix reactor in the side-stream to recover phosphorus from the bottom of the dewatering treatment unit. All other upgrading combinations involving chemical precipitation and Exelys technologies were not found economical for the given plant. Sensitivity analyses on the economic evaluation criteria have demonstrated that the results obtained are robust against uncertainties in influent wastewater characteristics and technical (e.g. recovery yield) performance parameters.

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.

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Research output: Research - peer-review > Article in proceedings – Annual report year: 2017

Uncertainty and Sensitivity Analysis for an Ibuprofen Synthesis Model Based on Hoechst Path
The pharmaceutical industry faces several challenges and barriers when implementing new or improving current pharmaceutical processes, such as competition from generic drug manufacturers and stricter regulations from the U.S. Food and Drug Administration, as well as 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 modelinterface. The process flowsheet is based on the Hoechst path, starting from the Friedel-Craftsacetylation of isobutylbenzene to 4-isobutylphenylacetophenone, its further hydrogenation to IBPE (1,4-isobutylphenylethanol) and the carbonylation to both ibuprofen and by-products. The integration of the referred models takes into account the different solvents used in reactions, as well as the presence of by-products and the irrations. 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 consists 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.

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Contributors: da Conceicao Do Carmo Montes, F., Gernaey, K. V., Sin, G.
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Uncertainty assessment of equations of state with application to an organic Rankine cycle

Evaluations of equations of state (EoS) should include uncertainty. This study presents a generic method to analyse EoS from a detailed uncertainty analysis of the mathematical form and the data used to obtain EoS parameter values. The method is illustrated by comparison of Soave–Redlich–Kwong (SRK) cubic EoS with perturbed-chain statistical associating fluid theory (PC-SAFT) EoS for an organic Rankine cycle (ORC) for heat recovery to power from the exhaust gas of a marine diesel engine using cyclopentane as working fluid. Uncertainties of the EoS input parameters including their corresponding correlation structure, are quantified from experimental measurements using a bootstrap method. Variance-based sensitivity analysis is used to compare the uncertainties from the departure function and the ideal-gas contribution. A Monte Carlo procedure propagates fluid parameter input uncertainty onto the model outputs. Uncertainties in the departure function (SRK or PC-SAFT EoS) dominate the total uncertainties of the ORC model output. For this application and working fluid, SRK EoS has less predictive uncertainty in the process model output than does PC-SAFT EoS, 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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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, National Institute of Standards and Technology, University of Virginia
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Web of Science (2017): Impact factor 1.704
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Web of Science (2016): Indexed yes
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Scopus rating (2015): CiteScore 1.68 SJR 0.729 SNIP 0.761
Web of Science (2015): Impact factor 1.837
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.48 SJR 0.693 SNIP 0.642
Web of Science (2014): Impact factor 1.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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Web of Science (2013): Impact factor 1.642
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.62 SJR 0.821 SNIP 0.731
Web of Science (2012): Impact factor 1.67
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.

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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.
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.

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Organisations: Department of Electrical Engineering, Automation and Control, Center for Electric Power and Energy, Energy System Management, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, China University of Mining And Technology
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A Comprehensive Methodology for Development, Parameter Estimation, and Uncertainty Analysis of Group Contribution Based Property Models - An Application to the Heat of Combustion

A rigorous methodology is developed that addresses numerical and statistical issues when developing group contribution (GC) based property models such as regression methods, optimization algorithms, performance statistics, outlier treatment, parameter identifiability, and uncertainty of the prediction. The methodology is evaluated through development of a GC method for the prediction of the heat of combustion (ΔHco) for pure components. The results showed that robust regression lead to best performance statistics for parameter estimation. The bootstrap method is found to be a valid alternative to calculate parameter estimation errors when underlying distribution of residuals is unknown. Many parameters (first, second, third order group contributions) are found unidentifiable from the typically available data, with large estimation error bounds and significant correlation. Due to this poor parameter identifiability issues, reporting of the 95% confidence intervals of the predicted property values should be mandatory as opposed to reporting only single value prediction, currently the norm in literature. Moreover, inclusion of higher order groups (additional parameters) does not always lead to improved prediction accuracy for the GC-models; in some cases, it may even increase the prediction error (hence worse prediction accuracy). However, additional parameters do not affect calculated 95% confidence interval. Last but not least, the newly developed GC model of the heat of combustion (ΔHco) shows predictions of great accuracy and quality (the most data falling 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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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 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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Web of Science (2013): Impact factor 4.538
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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.
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.
Control of wastewater $\text{N}_2\text{O}$ emissions by balancing the microbial communities using a fuzzy-logic approach

In this work, a fuzzy-logic controller for minimization of the nitrous oxide emission from wastewater treatment plants is developed and tested in a simulation environment. The controller is designed in order to maintain a balance between production and consumption of nitrite by AOB and NOB microorganisms respectively. Thus, accumulation of nitrite is prevented and AOB denitrification, the main $\text{N}_2\text{O}$ producer, is drastically slowed down. The controller is designed to adjust the oxygen supply according to a measured parameter which typically indicates the ratio of the activity of NOB over AOB.

The controller is tested on a benchmark simulation model describing the production of $\text{N}_2\text{O}$ during both AOB denitrification and HB denitrification. Comparisons between simulation results of open-loop and closed-loop have revealed the potential of the controller to significantly reduce the amount of $\text{N}_2\text{O}$ emitted (approximately 35%). On the other side, this reduction of $\text{N}_2\text{O}$ was accompanied by an increase in the aeration costs. Moreover, a plant performance evaluation under dynamic conditions has shown that the controller is able to adapt to changes in the operational conditions, thus maintaining the desired balance between production and consumption of nitrite.
disturbances shows that the effluent quality is compromised due to higher requirements of organic carbon by denitrifying heterotrophs. The controller can therefore be considered effective for the reduction of N$_2$O production by AOB but would need to be coupled with a secondary control strategy ensuring a complete oxidation of the nitrogen oxides by heterotrophs to have a good effluent quality.

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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 et al., 2010) and can be broadly defined as follows: Given a model and a set of data/measurements from the experimental setup in question, estimate all or some of the parameters of the model using an appropriate statistical method.

The focus of this chapter is to provide a set of tools and the techniques necessary to estimate the kinetic and stoichiometric parameters for wastewater treatment processes using data obtained from experimental batch activity tests. These methods and tools are mainly intended for practical applications, i.e. by consultants, engineers, and professionals. However, it is also expected that they will be useful both for graduate teaching as well as a stepping stone for academic researchers who wish to expand their theoretical interest in the subject. For the models selected to interpret the experimental data, this chapter uses available models from literature that are mostly based on the ActivatedSludge 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.

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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.

Economic risk analysis and critical comparison of optimal biorefinery concepts

In this paper, eight optimal biorefinery concepts for biofuels and biochemicals production are critically analyzed and compared in terms of their techno-economic performance and associated economic risks against historical market fluctuations. The investigated biorefinery concepts consider different combinations of biomass feedstock (lignocellulosic versus algal) and conversion technologies (biochemical versus thermochemical). In addition, the economic performance of each biorefinery concept is tested assuming a sudden drop in oil prices in order to compare the fitness/survival of each concept under extreme market disturbances. The analyses reveal amongst others that: (i) lignocellulosic bioethanol production is not economically feasible considering a drop in oil prices (a negative internal rate of return); (ii) a multi-product biorefinery concept, where bioethanol is upgraded to higher value-added chemicals (diethyl ether and 1,3-butadiene), provides an improved resilience and robustness against market price fluctuations by reducing economic loss by 140 MM$/a (17% IRR); (iii) the economic analysis favors biochemical conversion technologies for a small production/processing capacity, whereas the thermochemical conversion platform is favored for a relatively larger production capacity; and (iv) the microalgae-based biorefinery concept performed worse in terms of economics compared to the others, which is largely due to the cost of algae production and harvesting. In general, we recommend that a comprehensive economic risk analysis, using for example the 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 for chemicals and fuels.
Economic Risk Assessment of Early Stage Designs for Glycerol Valorization in Biorefinery Concepts

A systematic methodology to critically assess and screen among early stage design alternatives was developed for the use of glycerol. Through deterministic sensitivity analysis it was found that variations in the product and feedstock prices, total production cost, fixed capital investment, and discount rate, among others, have high impact on the project’s profitability analysis. Therefore, the profitability was tested under uncertainties by using NPV and MSP as economic metrics. The robust ranking of solutions is presented with respect to minimum economic risk of the project being nonprofitable (failure to achieve a positive NPV times the consequential profit loss). It was found that the best potential options for glycerol valorization is through the production of either (i) lactic acid (9 MM$ with 63% probability of failure to achieve a positive NPV); (ii) succinic acid (14 MM$ with 76%); or finally, (iii) 1,2-propanediol (16 MM$ with 68%). As a risk reduction strategy, a multiproduct biorefinery is suggested which is capable of switching between the production of lactic acid and succinic acid. This solution comes with increased capital investment; however, it leads to more robust NPV and decreased economic risk by approximately 20%, therefore creating a production plant that can continuously adapt to
market forces and thus optimize profitability.

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BFI (2015): BFI-level 2  
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BFI (2009): BFI-level 2  
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Web of Science (2009): Indexed yes
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.

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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.


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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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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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Scopus rating (2016): CiteScore 3.11 SJR 1.035 SNIP 1.29
Web of Science (2016): Impact factor 2.836
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.03 SJR 1.085 SNIP 1.428
Web of Science (2015): Impact factor 2.98
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.86 SJR 1.066 SNIP 1.337
Web of Science (2014): Impact factor 2.748
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.59 SJR 1.053 SNIP 1.355
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): CiteScore 2.46 SJR 0.98 SNIP 1.437
Web of Science (2012): Impact factor 2.493
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 (KLFL) between LFL and temperature is introduced and an MG GC model to estimate KLFL 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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BFI (2015): BFI-level 1
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Web of Science (2015): Impact factor 4.836
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BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.21 SJR 1.814 SNIP 2.258
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Group contribution modelling for the prediction of safety-related and environmental properties

We present a new set of property prediction models based on group contributions to predict major safety-related and environmental properties for organic compounds. The predicted list of properties includes lower and upper flammability limits, heat of combustion, auto ignition temperature, global warming potential and ozone depletion potential.

Process safety studies and environmental assessments rely on accurate property data. Safety data such as flammability
limits, heat of combustion or auto ignition temperature play an important role in quantifying the risk of fire and explosions among others. Global warming potential and ozone depletion potential became a standard to analyze the environmental impact of processes and products.

In the early stage of process development and analysis, experimental values are often not available due to cost or time constraints. In this case property prediction models like group contribution (GC) models can estimate data. However, the estimation needs to be accurate, reliable and as little time-consuming as possible so that the models can be used on the fly.

In this study the Marrero and Gani group contribution (MR GC) method has been used to develop the models for safety-related and environmental properties. The method considers the group contribution in three levels: The contributions from a specific functional group (1st order parameters), from poly-functional (2nd order parameters) as well as from structural groups (3rd order parameters). The latter two classes of GC factors provide additional structural information beside the functional group. The contributions of all three factors are then summed up. For the database, DIPPR are used together with the reported measurement accuracy. For parameter estimation, a comprehensive statistical methodology was followed to improve prediction accuracy and reliability (95% confidence).

The method is simple and easy to apply. Taking into account higher order groups increases the accuracy. Furthermore, the application range is high due to the high number of considered functional and structural contributions.

A thorough uncertainty analysis provides information about the prediction error, which is important for communicating the reliability of the predicted values for the user for potential applications in process safety studies and environmental assessments.

Example application of the models are shown for a selected class of chemicals to highlight the application range of models.
Modeling a production scale milk drying process: parameter estimation, uncertainty and sensitivity analysis

A steady state model for a production scale milk drying process was built to help process understanding and optimization studies. It involves a spray chamber and also internal/external fluid beds. The model was subjected to a comprehensive statistical analysis for quality assurance using sensitivity analysis of inputs/parameters, and uncertainty analysis to estimate confidence intervals on parameters and model predictions (error propagation). Variance based sensitivity analysis (Sobol's method) was used to quantify the influence of inputs on the final powder moisture as the model output. Bayesian inference using Markov Chain Monte Carlo sampling was used to quantify the uncertainty on the estimated parameters using available process data. In a full scale process the inputs with major range of variation are: moisture content at concentrate chamber feed (variation around 4%), and humidity at chamber inlet air (variation > 100%). The sensitivity analysis results suggest exploring improvements in the current control (Proportional Integral Derivative) for moisture content at concentrate chamber feed in order to reduce the output variance. It is also confirmed that humidity control at chamber inlet air stream would not be necessary because, despite its wide range of variation (air taken from outside), its impact on output variance is low. The uncertainty analysis results showed that confidence intervals obtained for parameters were reasonable, although some of them were found significantly correlated. For model applications, this means that model simulations should be performed using not only parameter values but also their correlation matrix by means of non-linear error propagation methods such as Monte Carlo techniques. The separate effects on model prediction uncertainties due to parameter estimation and measurement errors were studied. The results indicate that the error in measurements is the main responsible for the uncertainty in output predictions. Therefore using proper filtering of measurements, the comprehensively tested model is ready to support simulation based efforts for further process optimization. (C) 2016 Elsevier Ltd. All rights reserved.

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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 online monitoring tool.

The control strategy development follows on from the on-line model application. The aim of the control strategy is to maximise the total product achieved per batch. There is a demand to maximise the total product in each batch in industry, in order to meet increasing product demands with a limited capacity. The control algorithm is then defined in order to maximise the mass in the system, subject to the oxygen transfer rates in the system. Since the aim is to control to a target fill in a target time, a predictive model-based control algorithm is developed where by the model is simulated to the end of batch time at each model iteration. This provides a prediction of the future trajectory of the process, so that it is possible to guide the system to the desired target mass. The control strategy is applied on-line at 550L scale in the Novozymes A/S fermentation pilot plant, and the method is challenged with four different sets of process operating conditions. The controller reliably reaches the desired maximum tank fill, with a maximum error of under 5% of the target in eight experimental runs. The product concentration is not affected by the control strategy when compared to batches utilising a reference controller. This method has the benefit of reducing the variance in the final fill, which not only allows for a more reproducible product mass in a batch operation, but also aids downstream process scheduling and resource allocation activities in the industrial setting.

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Plant-wide modelling and control of nitrous oxide emissions from wastewater treatment plants
Nitrous oxide (N₂O) is a greenhouse gas with a global warming potential three hundred times stronger than carbon dioxide (CO₂). The IPCC report released in 2014 shows that the CO₂ equivalents emitted from the wastewater systems are increasing in the last decades. It was also estimated that 14% of those CO₂ equivalents comes from N₂O emissions. It becomes therefore relevant, within the context of reducing the carbon footprint of wastewater treatment (WWT) systems, to develop control strategies aimed at the minimization of the emissions of this gas. Till now, few operation strategies have been developed to reduce the amount of 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 \( \text{N}_2\text{O} \) predictions by the three models. Since there is at the moment no consensus model considered to describe reliably \( \text{N}_2\text{O} \) emissions from WWT plants, all the three models are used for testing the \( \text{N}_2\text{O} \) 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 \( \text{N}_2\text{O} \) 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 \( \text{N}_2\text{O} \) 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 \( \text{N}_2\text{O} \) emissions. The ratio between measured nitrate produced and ammonium consumed in the aerobic zone (\( \text{RNatAmm} \)) 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 \( \text{RNatAmm} \), \( \text{N}_2\text{O} \) 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 \( \text{N}_2\text{O} \) 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 \( \text{CO}_2 \) footprints of WWTPs.

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**Sources and propagation of uncertainty in \( \text{N}_2\text{O} \) model predictions**

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Synthesis of preliminary system designs for offshore oil and gas production

The present work deals with the design of oil and gas platforms, with a particular focus on the development of integrated and intensified petroleum processing plants. It builds on a superstructure based approach that includes all the process steps, transformations and interconnections of relevance, to generate and compare a large number of alternatives. The superstructure is formulated based on engineering knowledge and is coupled to process models developed in Aspen and Matlab, together with multi-objective optimisation routines and uncertainty assessments. It takes actual measurements from North Sea fields and three petroleum compositions as starting points. The significance of the uncertainties associated with the feed properties, and the capital costs, taxes and lifetime, is assessed. The results indicate that (i) the system performance strongly depends on the level of mass integration within the platform, (ii) the oil and gas recoveries are markedly impacted by the number of separation stages and heat exchangers, and (iii) disregarding the interactions between the several plant sections lead to sub-optimum solutions. The application of this framework proves to be useful for eliminating inadequate configurations and screening potentially novel solutions at early stage designs, with respect to technical, energetic and economic criteria.
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.

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Systematic design of optimal control systems for WWTPs: case study of the SHARON-Anammox process

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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 plants. Moreover, it will facilitate the development of strategies to minimize the carbon footprint of wastewater treatment plants.

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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.
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.

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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, nitratation, anaerobic ammonium oxidation and overall autotrophic nitrogen removal. These four results give insight into the state of the process and are used as inputs for the controller that manipulates the aeration to the reactor. The diagnosis tool was first evaluated using 100 days of real process operation data obtained from a lab-scale single-stage autotrophic nitrogen removing reactor. This evaluation revealed that the fuzzy logic diagnosis is able to provide a realistic description of the microbiological state of the reactor with process engineering insight analysis. An evaluation of both the diagnosis tool and the controller was done by simulating a disturbance in the influent concentration. High and steady nitrogen removal efficiency was achieved thanks to the diagnosis and control system. Finally, development of the diagnosis and control as two independent systems provided further insight into the operation performance, gives transparency towards the operator and makes the system flexible for future maintenance or improvements.
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 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 expected 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.
A mathematical programming framework for early stage design of wastewater treatment plants

The increasing number of alternative wastewater treatment technologies and stricter effluent requirements make the optimal treatment process selection for wastewater treatment plant design a complicated problem. This task, defined as wastewater treatment process synthesis, is currently based on expert decisions and previous experiences. This paper proposes a new approach based on mathematical programming to manage the complexity of the problem. The approach generates/identifies novel and optimal wastewater treatment process selection, and the interconnection between unit operations to create a process flow diagram. Towards this end, a superstructure approach is used to represent the treatment alternatives for reaction and separation. A generic process interval model is used to describe each alternative in terms of input/output mass balances including conversion and separation factors. Next the design problem is formulated as a Mixed Integer (Non)linear Programming problem and solved. A case study is formulated and solved to highlight the application of the framework. © 2014 Elsevier Ltd. All rights reserved.
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 PASST framework was presented that focuses on determining the potential for control in sewer system operation. However, for the actual design of control systems urban drainage planners still have to rely on their operational knowledge combined with model simulations and trial and error. This is an inefficient process where the final design largely depends on the urban drainage planner's knowledge about the system dynamics and control in general. The motivation for this thesis was therefore the wish for a methodological approach to sewer system control design. Using a case study the following research hypothesis was tested in this thesis:

Using classical and modern control theory, a methodological approach can be derived for designing sewer system control. This can aid urban drainage 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 theory for process control design can be applied
meaningfully to the sewer system. As the methodology takes its basis in a hierarchical decomposition of the control problem based on time-scale, it was also investigated if sewer system control can be decomposed in a similar manner. From a review of existing control systems for sewer systems in Europe, it was concluded that sewer system control can also be decomposed in a hierarchical manner based on differences in time-scale. The proposed time-scale dependent hierarchy for sewer system control contains four layers that each handles their own dedicated task. From the bottom and up they are: 1) the regulatory control layer, 2) the coordinating control layer, 3) the optimisation layer and 4) the management of objectives layer.

The time-scale dependent hierarchy for sewer system control is put into a framework that also contains a terminology related to control. In this way the Planning aid for sewer system real time control framework can help to compare different control system solutions and facilitate a clear communication between different professions and disciplines working together in sewer system control design.

Starting from the hierarchical decomposition of sewer system control in layers, a stepwise approach to design sewer system control was proposed and followed. The individual layers of the hierarchy were designed one by one for a case study in Copenhagen, with the methods and tools taken from both classical and modern control theory.

The tools of classical control theory are developed for systems that can be approximated by linear models. The main challenge of using classical control theory on the case study was therefore the transient nature and the non-linearity of the sewer system dynamics. The methodology was adapted, by linearizing the sewer system model at various points in time, creating a step-wise linear model. The results of the linearization showed that the sewer system dynamics could be divided into four phases, characterised by the following operation modes: dry weather, filling, saturation and emptying.

Having obtained a piece-wise linear model for each of the operational modes, the tools from classical control theory, such as the calculation of the condition number and the relative gain array, could be successfully applied to the sewer system. Based on the results a pairing between the measurements variables and the actuators could be suggested. Having proposed to decompose the sewer system control in a hierarchical manner, it became necessary to investigate the role of the lowest layer in the hierarchy, which is the regulatory control layer. Traditionally the role of the regulatory layer is to reject disturbances and track the setpoints, and the simplest form of regulatory control has just constant setpoints. However, in a transient system like the sewer system, the setpoints may change dramatically and rapidly. Therefore the regulatory control layer may not have the same functionality when designed for the sewer system. From the application of the classical control theory it was found that the system dynamics could be described by four operational modes, and instead of a fixed setpoint the regulatory control layer needs changing setpoints, according to the operational modes.

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.

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A novel control strategy for single-stage autotrophic nitrogen removal in SBR

A novel feedforward–feedback control strategy was developed for complete autotrophic nitrogen removal in a sequencing batch reactor. The aim of the control system was to carry out the regulation of the process while keeping the system close to the optimal operation. The controller was designed based on a process model and then tested experimentally. The resulting batch-to-batch control strategy had the total nitrogen removal efficiency as controlled variable and the setting of the aeration mass flow controller as manipulated variable. Compared to manual operation mode (constant air supply), the controller resulted in a significant performance improvement: removal efficiency was kept at a stable high level in the presence of influent ammonium concentration disturbances, and the absolute deviation on removal efficiency was reduced by 40%. The successful validation of the controller in a lab-scale reactor is a promising result, which brings this control strategy one step closer to full-scale implementation.

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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 data sampling 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.

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A rigorous methodology for development and uncertainty analysis of group contribution based property models

Property prediction models are a fundamental tool of process modeling and analysis, especially at the early stage of process development. Furthermore, property prediction models are the fundamental tool for Computer-aided molecular design used for the development of new refrigerants. Group contribution (GC) based prediction methods use structurally dependent parameters in order to determine the property of pure components. The aim of the GC parameter estimation is to find the best possible set of model parameters that fits the experimental data. In that sense, there is often a lack of attention on numerical and statistical challenges associated with model development and analysis. These challenges
include for example (i) performance of optimization algorithms used for finding minimum of the objective function for the parameter estimation, (ii) assessment of parameter estimation errors, (iii) 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 bootstrap 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.

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Challenges encountered calibrating N2O dynamics from mixed cultures

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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 limitations, as well as changes in the wastewater treatment trends, e.g. from nutrient removal to nutrient recovery. Similarly, recovery possibilities for clean water, energy and materials shifted the perception about wastewater towards being a valuable resource rather than being a waste. While the regulations change to impose stricter effluent limit values for the contaminants, the increasing population and the size of the cities put a barrier on the expansion of the existing WWTPs. Therefore, the retrofitting task has become a complex integrated decision making problem where a number of aspects have to be accounted for in the early stage decision making. 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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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: Import and 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.

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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°C 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.

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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 real-time 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.

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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.

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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).

Extending the benchmark simulation model nO2 with processes for nitrous oxide production and side-stream nitrogen removal

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.
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 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 Nitrosospira 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.

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.
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[2]. There is also a lack of sensors for key variables which are essential to define the operation[3], 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 high measurement noise. This requires additional preprocessing steps in order to extract the information within such a dataset. A 30 batch dataset from a production process operating at Novozymes A/S was 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.

Multivariate Analysis of Industrial Scale Fermentation Data

Multivariate analysis allows process understanding to be gained from the vast and complex datasets recorded from fermentation processes, however the application of such techniques to this field can be limited by the data pre-processing requirements and data handling. In this work many iterations of multivariate modelling were carried out using different data pre-processing and scaling methods in order to extract the trends from the industrial data set, obtained from a production process operating in Novozymes A/S. This data set poses challenges for data analysis, combining both online and offline variables, different data sampling intervals, and noise in the measurements, as well as different batch lengths. By applying unfold principal component regression (UPCR) and unfold partial least squares (UPLS) regression algorithms, the product concentration could be predicted for 30 production batches, with an average prediction error of 7.6%. A methodology is proposed for applying multivariate analysis to industrial scale batch process data.

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.

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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 WWTP process selection for treatment of domestic wastewater - A realistic full-scale retrofitting study

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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.

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 of organic chemicals. Furthermore, it provides a systematic method for outlier treatment in order 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.

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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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 cycledesigns 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 using 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-heat water stream at temperature 120°C and pressure 4 bar. Overall this contribution presents 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 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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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.

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**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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Systematic network synthesis and design: Problem formulation, superstructure generation, data management and solution

The developments obtained in recent years in the field of mathematical programming considerably reduced the computational time and resources needed to solve large and complex Mixed Integer Non Linear Programming (MINLP) problems. Nevertheless, the application of these methods in industrial practice is still limited by the complexity associated with the mathematical formulation of some problems. In particular, the tasks of design space definition and representation as superstructure, as well as the data collection, validation and handling may become too complex and cumbersome to execute, especially when large problems are considered. In an earlier work, we proposed a computer-aided framework for synthesis and design of process networks. In this contribution, we expand the framework by including methods and tools developed to structure, automate and simplify the mathematical formulation of the design problem. Furthermore, the models employed for the representation of the process alternatives included in the superstructure are refined, through the inclusion of the energy balance. Finally, the features of the framework are highlighted through the solution of two case studies focusing on food processing and biofuels.

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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.

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.
Upgrading of lignocellulosic biorefinery to value-added chemicals: Sustainability and economics of bioethanol-derivatives

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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Utrecht University
Contributors: Cheali, P., Posada, J. A., Gernaey, K., Sin, G.
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Publication information
Journal: Biomass & Bioenergy
Volume: 75
ISSN (Print): 0961-9534
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4 SJR 1.235 SNIP 1.436
Web of Science (2017): Impact factor 3.358
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.198 SNIP 1.385
Web of Science (2016): Impact factor 3.219
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.03 SJR 1.51 SNIP 1.596
Web of Science (2015): Impact factor 3.249
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.36 SJR 1.865 SNIP 1.964
Web of Science (2014): Impact factor 3.394
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Electrical Engineering, Automation and Control, Center for Electric Power and Energy, Energy System Management, CAPEC-PROCESS
Contributors: Wu, J., Lind, M., Zhang, X., Jørgensen, S. B., Sin, G.
Pages: 293-298
Publication date: 2015

Host publication information
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Volume: 37
Publisher: Elsevier
Editors: Gernaey, K. V., Huusom, J. K., Gani, R.
(Keywords: Functional Model, Multilevel Flow Modeling, Model Validation, Process Safety)
Research output: Research - peer-review › Article in proceedings – Annual report year: 2015

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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Illinois at Chicago
Contributors: Heitzig, M., Linninger, A., Sin, G., Gani, R.
Number of pages: 22
Pages: 677–698
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Computers & Chemical Engineering
Volume: 71
ISSN (Print): 0098-1354
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
Web of Science (2017): Impact factor 3.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1 SNIP 1.631
Web of Science (2016): Impact factor 3.024
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.713
Web of Science (2015): Impact factor 2.581
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.22 SJR 1.168 SNIP 1.728
Web of Science (2014): Impact factor 2.784
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.06 SJR 1.21 SNIP 1.744
Web of Science (2013): Impact factor 2.452
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.05 SJR 1.138 SNIP 1.897
Web of Science (2012): Impact factor 2.091
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.8 SJR 1.144 SNIP 1.736
Web of Science (2011): Impact factor 2.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.167 SNIP 1.752
Web of Science (2010): Impact factor 2.072
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.171 SNIP 2.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.288 SNIP 2.094
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.621 SNIP 1.916
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.306 SNIP 1.888
Scopus rating (2005): SJR 1.306 SNIP 1.882
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.112 SNIP 1.86
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.332 SNIP 1.884
Scopus rating (2002): SJR 0.8 SNIP 0.916
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.951 SNIP 0.745
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.125 SNIP 1.054
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.05 SNIP 1.131
Original language: English
Keywords: Computer-aided modelling framework, Pharmacokinetics, Physiologically-based pharmacokinetic, Modelling, Model identification, Modelling software, Sensitivity analysis
DOIs: 10.1016/j.compchemeng.2014.07.016
Source: PublicationPreSubmission
Source-ID: 101104828
Research output: Research - peer-review ; Journal article – Annual report year: 2014
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for BioProcess Engineering
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Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Applied Biochemistry and Biotechnology
Volume: 172
Issue number: 6
ISSN (Print): 0273-2289
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.02 SJR 0.571 SNIP 0.8
Web of Science (2017): Impact factor 1.797
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.81 SJR 0.579 SNIP 0.749
Web of Science (2016): Impact factor 1.751
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.67 SJR 0.575 SNIP 0.736
Web of Science (2015): Impact factor 1.606
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.92 SJR 0.644 SNIP 0.94
Web of Science (2014): Impact factor 1.735
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.18 SJR 0.747 SNIP 1.027
Web of Science (2013): Impact factor 1.687
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
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.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University of Virginia
Contributors: Anantpinijwatna, A., Sin, G., O’Connell, J. P., Gani, R.
Pages: 249-254
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Title of host publication: Proceedings of the 8th International Conference on Foundations of Computer-Aided Process Design
Publisher: Elsevier
ISBN (Print): 978-0-444-63433-7
(Keywords: Biphasic reacting system, Modelling, Phase transfer catalyst, Benzoin condensation)

**Research output:** Research - peer-review → Article in proceedings – Annual report year: 2014

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An integrated approach for synthesis and design of process and water/wastewater networks

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Handani, Z. B., Quaglia, A., Sin, G., Gani, R.
Publication date: 2014
Peer-reviewed: Yes
Event: Abstract from 21st International Congress of Chemical and Process Engineering, Prague, Czech Republic.
Source: PublicationPreSubmission
Source-ID: 103645959

**Research output:** Research - peer-review → Conference abstract for conference – Annual report year: 2014

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An integrated qualitative and quantitative modeling framework for computer-assisted HAZOP studies

The article proposes a novel practical framework for computer-assisted hazard and operability (HAZOP) that integrates qualitative reasoning about system function with quantitative dynamic simulation in order to facilitate detailed specific HAZOP analysis. The practical framework is demonstrated and validated on a case study concerning a three-phase separation process. The multilevel flow modeling (MFM) methodology is used to represent the plant goals and functions. First, means-end analysis is used to identify and formulate the intention of the process design in terms of components, functions, objectives, and goals on different abstraction levels. Based on this abstraction, qualitative functional models are constructed for the process. Next MFM-specified causal rules are extended with systems specific features to enable proper reasoning. Finally, systematic HAZOP analysis is performed to identify safety critical operations, its causes and consequences. The outcome is a qualitative hazard analysis of selected process deviations from normal operations and their consequences as input to a traditional HAZOP table. The list of unacceptable high risk deviations identified by the qualitative HAZOP analysis is used as input for rigorous analysis and evaluation by the quantitative analysis part of the framework. To this end, dynamic first-principles modeling is used to simulate the system behavior and thereby complement the results of the qualitative analysis part. The practical framework for computer-assisted HAZOP studies introduced in this article allows the HAZOP team to devote more attention to high consequence hazards. © 2014 American Institute of Chemical Engineers AIChE J 60: 4150–4173, 2014

**General information**
State: Published
Organisations: Department of Electrical Engineering, Automation and Control, Center for Electric Power and Energy, Energy System Management, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Safepark Consultancy, China University of Petroleum
Pages: 4150-4173
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: AIChE Journal
Volume: 60
Issue number: 12
An Integrated Systematic Framework to Assist the Development of Pharmaceutical Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Papadakis, E., Sin, G., Gernaey, K., Gani, R.
Number of pages: 2
Publication date: 2014
Peer-reviewed: Yes
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Electronic versions:
An_integrated_systematic_framework.pdf

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 limitations, 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 balance. 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
Contributors: Bozkurt, H., Quaglia, A., Gernaey, K., Sin, G.
Number of pages: 4
Publication date: 2014

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Title of host publication: Proceedings of 2nd IWA Specialized Conference on Eco-technologies for Sewage Treatment Plants
Keywords: Design, Modelling, Superstructure optimization, Uncertainty analysis, Wastewater treatment
Source: PublicationPreSubmission
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 crystallization operation for the paracetamol-ethanol system.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Fedorova, M., Papadakis, E., Meisler, K. T., Sin, G., Gani, R.
Pages: 309-314
Publication date: 2014

Host publication information
Title of host publication: Proceedings of the 8th International Conference on Foundations of Computer-Aided Process Design
Volume: 34
Publisher: Elsevier
ISBN (Print): 978-0-444-63433-7
(Computer Aided Chemical Engineering, Vol. 34).
Keywords: Modeling framework, Computer-aided template, Oxidation of unsaturated fatty acid, Crystallization
DOI: 10.1016/b978-0-444-63433-7.50036-5

Research output: Research - peer-review › Article in proceedings – Annual report year: 2014

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Handani, Z. B., Quaglia, A., Sin, G., Gani, R.
Publication date: 2014
Peer-reviewed: Yes
Event: Abstract from 21st International Congress of Chemical and Process Engineering, Prague, Czech Republic.
Source: PublicationPreSubmission
Source-ID: 103645951

Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2014
A Simultaneous Optimization Approach for Synthesis and Design of Process and Water Networks

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Handani, Z. B., Quaglia, A., Sin, G., Gani, R.
Publication date: 2014
Peer-reviewed: Yes
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2014

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
Publication date: 2014
Peer-reviewed: Yes
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.

Bibliographical note
ORAL PRESENTATION
Source: PublicationPreSubmission
Source-ID: 103645239
Research output: 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
Contributors: Fedorova, M., Sin, G., Gani, R.
Pages: 817-822
Publication date: 2014

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Title of host publication: Proceedings of the 24th European Symposium on Computer Aided Process Engineering
Volume: 33
Publisher: Elsevier
Keywords: Modeling framework, Computer-aided template, Catalytic fixed bed reactor
DOIs:
10.1016/b978-0-444-63456-6.50137-x
Source: PublicationPreSubmission
Source-ID: 102119569
Research output: Research - peer-review › Article in proceedings – Annual report year: 2014

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Cheali, P., Gernaey, K., Sin, G.
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 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 xyloooligomers 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.
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
Contributors: Bozkurt, H., Quaglia, A., Gernaey, K., Sin, G.
Pages: 254-257
Publication date: 2014

Host publication information
Title of host publication: Proceedings for of 4th IWA/WEF Wastewater Treatment Modelling Seminar
Research output: Research - peer-review › Article in proceedings – Annual report year: 2014

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
Contributors: Cheali, P., Quaglia, A., Gernaey, K. V., Sin, G.
Pages: 6021-6032
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 53
Issue number: 14
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
Web of Science (2017): Impact factor 3.141
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.87 SJR 0.938 SNIP 1.145
Web of Science (2015): Impact factor 2.567
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.85 SJR 1.009 SNIP 1.287
Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.6 SJR 0.975 SNIP 1.232
Web of Science (2013): Impact factor 2.235
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.56 SJR 1.054 SNIP 1.32
Web of Science (2012): Impact factor 2.206
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.58 SJR 1.076 SNIP 1.236
Web of Science (2011): Impact factor 2.237
ISI indexed (2011): ISI indexed yes
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.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Quaglia, A., Sin, G., Gani, R.
Number of pages: 6
Publication date: 2014

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Keywords: Synthesis and design of processing network, Capital budgeting, Mixed Integer Non Linear Programming, Financial optimization
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.

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
Contributors: Quaglia, A., Pennati, A., Bogataj, M., Kravanja, Z., Sin, G., Gani, R.
Number of pages: 12
Pages: 5160−5171
Publication date: 2014
Peer-reviewed: Yes

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.
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 crystalized 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.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Residual Resource Engineering, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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.
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.358
Web of Science (2017): Impact factor 7.051
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.49 SJR 2.663 SNIP 2.563
Web of Science (2016): Impact factor 6.942
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.63 SJR 2.665 SNIP 2.482
Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.13 SJR 2.946 SNIP 2.702
Web of Science (2014): Impact factor 5.528
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.02 SJR 2.956 SNIP 2.676
Web of Science (2013): Impact factor 5.323
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.15 SJR 2.914 SNIP 2.442
Web of Science (2012): Impact factor 4.655
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.43 SJR 2.862 SNIP 2.355
Web of Science (2011): Impact factor 4.865
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.592 SNIP 2.192
Web of Science (2010): Impact factor 4.546
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.319 SNIP 2.224
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.073 SNIP 2.178
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.94 SNIP 2.184
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.902 SNIP 2.233
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.113 SNIP 2.334
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.209 SNIP 2.108
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.702 SNIP 1.908
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.568 SNIP 1.757
Web of Science (2002): Indexed yes
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
Contributors: Bozkurt, H., Quaglia, A., Gernaey, K., Sin, G.
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Peer-reviewed: Yes

Publication information
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Volume: 33
ISSN (Print): 1570-7946
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.5 SJR 0.19 SNIP 0.251
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.48 SJR 0.207 SNIP 0.242
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.39 SJR 0.271 SNIP 0.283
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.4 SJR 0.255 SNIP 0.256
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.28 SJR 0.235 SNIP 0.208
ISI indexed (2013): ISI indexed no
Scopus rating (2012): CiteScore 0.33 SJR 0.206 SNIP 0.285
ISI indexed (2012): ISI indexed no
Scopus rating (2011): CiteScore 0.3 SJR 0.205 SNIP 0.261
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.218 SNIP 0.177
Scopus rating (2009): SJR 0.199 SNIP 0.252
Scopus rating (2008): SJR 0.2 SNIP 0.178
Scopus rating (2007): SJR 0.241 SNIP 0.171
Superstructure development and optimization under uncertainty for design and 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 and solve it to determine the optimal process selection and flow diagram that meets 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
Contributors: Bozkurt, H., Quaglia, A., Gernaey, K., Sin, G.
Number of pages: 6
Publication date: 2014

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Publisher: Elsevier
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Source: PublicationPreSubmission
Source-ID: 103645718
Research output: Research - peer-review › Conference article – Annual report year: 2014

Synthesis and design of hybrid biorefinery systems: a structural optimisation approach and uncertainty analysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Contributors: Cheali, P., Quaglia, A., Gernaey, K., Sin, G.
Publication date: 2014
Peer-reviewed: Yes
Event: Abstract from 21st International Congress of Chemical and Process Engineering, Prague, Czech Republic.

Bibliographical note
Oral presentation.
Source: PublicationPreSubmission
Source-ID: 103645148
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2014

The Ontology System for Easy and Reusable Model Knowledge Representation

General information
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Cheali, P., Gernaey, K., Sin, G.
Pages: 19-29
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: A C S Sustainable Chemistry & Engineering
Volume: 2
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.45 SJR 1.657 SNIP 1.369
Web of Science (2017): Impact factor 6.14
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.92 SJR 1.572 SNIP 1.434
Web of Science (2016): Impact factor 5.951
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 5.39 SJR 1.389 SNIP 1.353
Web of Science (2015): Impact factor 5.267
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.3 SJR 1.218 SNIP 1.188
Web of Science (2014): Impact factor 4.642
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Web of Science (2013): Impact factor
ISI indexed (2013): ISI indexed no
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.
Uncertainty and Sensitivity Analysis in Sustainable Process Design – Environmental Indicators

General information
State: Published
Organisations: CAPEC-PROCESS, Department of Chemical and Biochemical Engineering
Contributors: Loureiro da Costa Lira Gargalo, C., Sin, G.
Publication date: 2014
Peer-reviewed: Yes
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.

Bibliographical note
ORAL PRESENTATION
Source: PublicationPreSubmission
Source-ID: 103645283
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2014

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, BIOFOS Renseanlæg Lynetten, HOFOR A/S
Contributors: Mollerup, A. L., Thornberg, D., Mikkelsen, P. S., Johansen, N. B., Sin, G.
Number of pages: 4
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from 11th IWA conference on instrumentation control and automation, Narbonne, France.
Electronic versions:
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Source: PublicationPreSubmission
Source-ID: 133795269
Research output: Research - peer-review › Conference abstract for conference – 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
Contributors: Mauricio Iglesias, M., Sin, G.
Publication date: 2013
Peer-reviewed: Yes
Event: Poster session presented at 9th World Congress of Chemical Engineering Incorporating 15th Asian Pacific Confederation of Chemical Engineering Congress, Seoul, Korea, Republic of.
Source: dtu
Source-ID: u::9039
Research output: Research - peer-review › Poster – Annual report year: 2013
A computer-aided support tool for synthesis and design of biorefinery networks under uncertainty

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Cheali, P., Gernaey, K., Sin, G.
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from SCPPE 2013, Dalian, China.
Source: dtu
Source-ID: u::9018
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

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
Contributors: Mauricio Iglesias, M., Vangsgaard, A. K., Gernaey, K., Sin, G.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Poster session presented at CAB 2013, Mumbai, India.
Research output: Research - peer-review › Poster – 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.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Contributors: Mauricio Iglesias, M., Vangsgaard, A. K., Gernaey, K., Sin, G.
Pages: 205-210
Publication date: 2013

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Publisher: Elsevier
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(ISIFAC Proceedings Volumes (IFAC-PapersOnline), Vol. 12).
Keywords: Fuzzy logic, Control, Diagnosis, Biological wastewater treatment, Nitrogen removal
Research output: Research - peer-review › Article in proceedings – Annual report year: 2013

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 ($\Delta f^\circ H^\circ_{\text{gas}}$) 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 $\Delta f^\circ H^\circ_{\text{gas}}$ 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 $\Delta f^\circ H^\circ_{\text{gas}}$ 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 $\Delta f^\circ H^\circ_{\text{gas}}$ 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 $\Delta f^\circ H^\circ_{\text{gas}}$ provides significant improvement in accuracy with an average absolute error of 1.75kJ/mol and standard deviation of 2.61kJ/mol.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, DSM Food Specialties  
Contributors: Hukkerikar, A., Meier, R. J., Sin, G., Gani, R.  
Pages: 23-32  
Publication date: 2013  
Peer-reviewed: Yes

**Publication information**

Journal: Fluid Phase Equilibria  
Volume: 348  
ISSN (Print): 0378-3812  
Ratings:  
BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Scopus rating (2017): CiteScore 2.22 SJR 0.95 SNIP 1.033  
Web of Science (2017): Impact factor 2.197  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 2.33 SJR 0.85 SNIP 1.187  
Web of Science (2016): Impact factor 2.473  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): CiteScore 1.99 SJR 0.866 SNIP 0.998  
Web of Science (2015): Impact factor 1.846  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): CiteScore 2.28 SJR 0.981 SNIP 1.232  
Web of Science (2014): Impact factor 2.2  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): CiteScore 2.31 SJR 1.001 SNIP 1.277  
Web of Science (2013): Impact factor 2.241  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): CiteScore 2.31 SJR 1.151 SNIP 1.279  
Web of Science (2012): Impact factor 2.379  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): CiteScore 2.26 SJR 1.03 SNIP 1.235  
Web of Science (2011): Impact factor 2.139  
ISI indexed (2011): ISI indexed yes
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 autotrophic nitrogen removal process. The model based multiobjective scaleup offers a promising improvement compared to the rule of thumbs based empirical scale up rules.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Contributors: Mauricio Iglesias, M., Sin, G.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Source: dtu
Source-ID: u::8403
Research output: Research - peer-review › Poster – Annual report year: 2013
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Quaglia, A., Sin, G., Gani, R.
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Publication date: 2013
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Source: dtu
Source-ID: u::9436
Research output: Research - peer-review › Poster – Annual report year: 2013

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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Contributors: Quaglia, A., Gani, R., Sin, G., Sarup, B.
Number of pages: 239
Publication date: 2013

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Alberto Quaglia_PEC13-41.pdf

Bibliographical note
Source: dtu
Source-ID: u::9558
Research output: Research › Ph.D. thesis – Annual report year: 2013
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.

General information
State: Published
Organisations: Department of Environmental Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
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Peer-reviewed: Yes

Publication information
Journal: Water Science and Technology
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Web of Science (2012): Impact factor 1.102
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.25 SJR 0.594 SNIP 0.631
Web of Science (2011): Impact factor 1.122
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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.

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, Computer Aided Process Engineering Center, Lund University
Pages: 137–166
Publication date: 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
Contributors: Abdul Samad, N. A. F. B., Sin, G., Gernaey, K., Gani, R.
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 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
Contributors: Abdul Samad, N. A. F. B., Sin, G., Gernaey, K., Gani, R.
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Publication date: 2013
Peer-reviewed: Yes
Ratings:

- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
- Web of Science (2017): Impact factor 3.113
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.39 SJR 1 SNIP 1.631
- Web of Science (2016): Impact factor 3.024
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.713
- Web of Science (2015): Impact factor 2.581
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): CiteScore 3.22 SJR 1.168 SNIP 1.728
- Web of Science (2014): Impact factor 2.784
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): CiteScore 3.06 SJR 1.21 SNIP 1.744
- Web of Science (2013): Impact factor 2.452
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): CiteScore 3.05 SJR 1.138 SNIP 1.897
- Web of Science (2012): Impact factor 2.091
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): CiteScore 2.8 SJR 1.144 SNIP 1.736
- Web of Science (2011): Impact factor 2.32
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.167 SNIP 1.752
- Web of Science (2010): Impact factor 2.072
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.171 SNIP 2.137
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 1.288 SNIP 2.094
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.621 SNIP 1.916
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.306 SNIP 1.888
- Scopus rating (2005): SJR 1.306 SNIP 1.882
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.112 SNIP 1.86
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 1.332 SNIP 1.884
- Scopus rating (2002): SJR 0.8 SNIP 0.916
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
Contributors: Abdul Samad, N. A. F. B., Meisler, K. T., Sin, G., Gernaey, K., Gani, R.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from BIWIC 2013, Odense, Denmark.
Source: dtu
Source-ID: u::7430
Research output: Research - peer-review › Journal article – Annual report year: 2013

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 problems. Tools for the analysis of the uncertainty, 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.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
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Publication information
Journal: Computers & Chemical Engineering
Volume: 59
ISSN (Print): 0098-1354
Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
Web of Science (2017): Impact factor 3.113
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.

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 stepwise 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.
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.73 SJR 0.766 SNIP 0.933
Web of Science (2017): Impact factor 2.587
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.94 SJR 0.854 SNIP 1.132
Web of Science (2016): Impact factor 3.135
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.55 SJR 0.795 SNIP 0.952
Web of Science (2015): Impact factor 2.738
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.49 SJR 0.938 SNIP 1.023
Web of Science (2014): Impact factor 2.349
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.82 SJR 1.028 SNIP 1.191
Web of Science (2013): Impact factor 2.494
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.58 SJR 1.108 SNIP 1.161
Web of Science (2012): Impact factor 2.504
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.28 SJR 0.981 SNIP 0.96
Web of Science (2011): Impact factor 2.168
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.892 SNIP 0.905
Web of Science (2010): Impact factor 1.818
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.842 SNIP 0.948
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.808 SNIP 1.022
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.639 SNIP 0.845
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.674 SNIP 0.912
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.599 SNIP 0.941
Scopus rating (2004): SJR 0.645 SNIP 0.77
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.556 SNIP 1.104
Scopus rating (2002): SJR 0.686 SNIP 1.091
Scopus rating (2001): SJR 0.637 SNIP 0.983
Scopus rating (2000): SJR 0.639 SNIP 1.03
Scopus rating (1999): SJR 0.637 SNIP 1.075
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.
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Fedorova, M., Sin, G., Gani, R.
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Publication date: 2013

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Title of host publication: Proceedings of the 23rd European Symposium on Computer Aided Process Engineering – ESCAPE 23
Publisher: Elsevier
Keywords: Modeling framework, Fixed bed reactor, Computer-aided modeling.
Source: dtu
Source-ID: u::8705
Research output: Research - peer-review → Article in proceedings – 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
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Mauricio Iglesias, M., Huusom, J. K., Sin, G.
Pages: 60- 70
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Peer-reviewed: Yes

Publication information
Journal: Chemical Engineering and Processing
Volume: 67
ISSN (Print): 0255-2701
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.09 SJR 0.872 SNIP 1.344
Web of Science (2017): Impact factor 2.826
Web of Science (2017): 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.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Department of Environmental Engineering
Contributors: Vangsgaard, A. K., Mauricio Iglesias, M., Gernaey, K., Smets, B. F., Sin, G.
Pages: 769-774
Publication date: 2013

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Publisher: Elsevier
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Reviewed Conference proceeding
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Research output: Research - peer-review › Article in proceedings – Annual report year: 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, Department of Environmental Engineering
Contributors: Vangsgaard, A. K., Mauricio Iglesias, M., Gernaey, K., Smets, B. F., Sin, G.
Publication date: 2013
Bibliographical note
Oral conference presentation.
Number of pages: 1
Source: dtu
Source-ID: u::9038
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

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
Contributors: Mollerup, A. L., Mikkelsen, P. S., Johansen, N. B., Thornberg, D., Sin, G.
Publication date: 2013
Event information
Event: 2012 IWA World Water Congress and Exhibition
Location: Busan, Korea, Republic of
Research output: Research - peer-review › Sound/Visual production (digital) – 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
Contributors: Sin, G., Gani, R., Dam-Johansen, K.
Pages: 54-59
Publication date: 2013
Peer-reviewed: Yes
Publication information
Journal: Chemical Engineering Progress
Volume: 109
Issue number: 2
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.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Abdul Samad, N. A. F. B., Sin, G.
Pages: 207-212
Publication date: 2013

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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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
Pages: 661-666
Publication date: 2013

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
Contributors: Bozkurt, H., Quaglia, A., Gernaey, K., Sin, G.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Event: Abstract from Asset management for enhancing energy efficiency in water and wastewater systems, Marbella, Spain.
Keywords: Superstructure optimization, Modelling, Wastewater treatment
Source: dtu
Source-ID: u::9028
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

**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. 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**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
Contributors: Hukkerikar, A. S., Sin, G., Abildskov, J., Sarup, B., Gani, R.
Number of pages: 289
Publication date: 2013

**Publication information**
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Publisher: Technical University of Denmark, Department of Chemical and Biochemical Engineering
ISBN (Print): 978-87-93054-11-0
Driving towards stratified aggregation in single-stage nitritation/anammox reactors by varying aeration regimes

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering, Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Publication date: 2013
Peer-reviewed: Yes
Event: Poster session presented at IWA 9th international Conference on Biofilm Reactors, Paris, France.
Source: dtu
Source-ID: u::9138
Research output: Research - peer-review › Poster – Annual report year: 2013

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
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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.

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**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 list of alternatives and connections between them), ii) each of the process alternatives (in term 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 results 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.

**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.

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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.

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**Bibliographical note**
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.

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Scopus rating (2010): SJR 1.961 SNIP 1.92
Modeling, Experimentation, and Control of Autotrophic Nitrogen Removal in Granular Sludge Systems

Complete autotrophic nitrogen removal (CANR) is a novel process that can increase the treatment capacity for wastewaters containing high concentrations of nitrogen and low organic carbon to nitrogen ratios, through an increase of the volumetric removal rate by approximately five times. This process is convenient for treating anaerobic digester liquor, landfill leachate, or special industrial wastewaters, because costs related to the need for aeration and carbon addition are lowered by 60% and 100%, respectively, compared to conventional nitrification denitrification treatment. Energy and capital costs can further be reduced by intensifying the process and performing it in a single reactor, where all processes take place simultaneously, e.g. in a granular sludge reactor, which was studied in this project. This process intensification means on the other hand an increased complexity from an operation and control perspective, due to the smaller number of actuators available.

In this work, an integrated modeling and experimental approach was used to improve the understanding of the process, and subsequently use this understanding to design novel control strategies, providing alternatives to the current ones available. First, simulation studies showed that the best removal efficiency was almost linearly dependent on the volumetric oxygen to nitrogen loading ratio. This finding among others, along with experimental results from start-up of lab-scale reactors, served as the basis for development of three single-loop control strategies, having oxygen supply as the actuator and removal efficiency as the controlled variable. These were investigated through simulations of an experimentally calibrated and validated model. A feedforward-feedback control strategy was found to be the most versatile towards the disturbances at the expense of slightly slower dynamic responses and additional complexity of the control structure. The functionality of this strategy was tested experimentally in a lab-scale reactor, where it showed the ability to reject disturbances in the incoming ammonium concentrations. However, during high ammonium loadings, when the capacity of the present sludge was reached, an oscillatory response was observed. Proper tuning of the controller is therefore of essential importance.

In this thesis, it was demonstrated that proactive use of model simulations, in an integrated methodology with experimentation, resulted in improved process understanding and novel control ideas. This will contribute to moving this promising technology from a case-by-case ad hoc approach to a more systematic knowledge based approach.
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.

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 N$_2$O 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 crystalized 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 N$_2$O production during wastewater treatment.

Molecular structure based property modeling: Development/improvement of property models through a systematic property-data-model analysis

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.

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**Performance of an autotrophic nitrogen removing reactor: Diagnosis through fuzzy logic**

Autotrophic nitrogen removal through nitritation-anammox in one stage SBRs is an energy and cost efficient alternative to conventional treatment methods. Intensification of an already complex biological system challenges our ability to observe, understand, diagnose, and control the system. A fuzzy logic diagnosis tool was developed, utilizing stoichiometric and concentration ratio measurements and removal efficiencies, along with rules derived from process knowledge. The tool could accurately determine the overall performance of the system and can therefore serve as a powerful tool to provide input for future control applications.

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**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 nitritation-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.

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Scopus rating (2008): SJR 0.583 SNIP 0.694
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Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.696 SNIP 0.789
Web of Science (2006): 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.

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Selection of controlled variables in bioprocesses. Application to a SHARON-Anammox 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-Anammox process for autotrophic nitrogen removal.

General information
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.

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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.

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Superstructure development and optimization for design/retrofit of municipal wastewater treatment plants
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
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 a large number of alternatives at their optimal points. In this study, the superstructure for thermochemical conversion routes 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 combinations 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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Cheali, P., Gernaey, K., Sin, G.
Number of pages: 6
Publication date: 2013
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Event: Poster session presented at 23rd European Symposium on Computer Aided Process Engineering, Lappeenranta, Finland.
Source: dtu
Source-ID: u::8703
Research output: Research - peer-review › Article in proceedings – Annual report year: 2013

Synthesis and design of future biorefineries with multi-criteria evaluation (technical and economic feasibility, environmental impact and sustainability).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Cheali, P., Gernaey, K., Sin, G.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Source: dtu
Source-ID: u::9465
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013
Synthesis and Design of Thermochemical and Biochemical Biomass Processing Networks under Uncertainty

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Cheali, P., Gernaey, K., Sin, G.
Number of pages: 1
Publication date: 2013
Peer-reviewed: Yes
Electronic versions:
ECCE-9_pche_abstract.pdf

Bibliographical note
Oral presentation
Source: dtu
Source-ID: u::8401

Uncertainty and Sensitivity Analysis on PAT System Performance for Crystallization Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Abdul Samad, N. A. F. B., Sin, G., Gernaey, K., Gani, R.
Number of pages: 2
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Peer-reviewed: Yes
Keywords: Crystallization, PAT system, Uncertainty analysis, Sensitivity analysis
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Source: dtu
Source-ID: u::9041

Use of continuous lactose fermentation for ethanol production by Kluyveromyces 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 Kluyveromyces 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 Ytrue sx = 0.114, Ytrue ex = 0.192 and Ysg = 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
Contributors: Sansonetti, S., Hobley, T. J., Curcio, S., Villadsen, J., Sin, G.
Pages: 703-709
Publication date: 2013
Peer-reviewed: Yes
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.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Center for Process Engineering and Technology
Contributors: Morales Rodriguez, R., Meyer, A. S., Gernaey, K., Sin, G.
Pages: 115-129
Publication date: 2012
Peer-reviewed: Yes

Publication information

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
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center,
Center for Process Engineering and Technology
Contributors: Abdul Samad, N. A. F. B., Meisler, K. T., Sin, G., Gernaey, K., Gani, R.
Publication date: 2012
Peer-reviewed: No
Keywords: Process monitoring and control, Analytical estimator, Crystal distribution, Crystal shape

Bibliographical note
Oral presentation.

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828-843.
Source: dtu
Source-ID: u::4423
Research output: Research › Conference abstract for conference – Annual report year: 2012

A Model-Based and a Multi-Objective Optimisation Framework for Incremental Scale-Up of Bioreactors

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Mauricio Iglesias, M., Sin, G.
Publication date: 2012
Peer-reviewed: Yes
Electronic versions:
AIChE_Paper 211g.pdf
URLs:
https://aiche.confex.com/aiche/2012/webprogram/Paper278274.html

Bibliographical note
Poster presentation.
Source: dtu
Source-ID: u::5327
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2012

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).

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Sin, G.
Number of pages: 15
Publication date: 2012
Peer-reviewed: No
Electronic versions:

**Abstract**

**Bibliographical note**

Oral presentation

Source: dtu

**Research output:** Research – Annual report year: 2012

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**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
Number of pages: 5
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Publication date: 2012

**Host publication information**

Title of host publication: Proceedings of IWA World Water Congress & Exhibition
Keywords: Decision-making, Autotrophic nitrogen removal, Stoichiometry, Anammox
Source: dtu
Source-ID: u::5197
Research output: Research - peer-review › Article in proceedings – Annual report year: 2012

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**An operation protocol for facilitating start-up of single-stage autotrophic nitrogen removing reactors based on process stoichiometry**

**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 information**

Event: 2012 IWA World Water Congress and Exhibition
Location: Busan, Korea, Republic of

**Bibliographical note**

Oral presentation.
Number of pages: 21
Source: dtu
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 gasreinjection process model as case study.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, DONG Energy AS, Kongsberg Maritime, Maersk Oil
Contributors: Enemark-Rasmussen, R., Cameron, D., Angelo, P. B., Sin, G.
Pages: 1271-1275
Publication date: 2012

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
Contributors: Quaglia, A., Pennati, A., Sin, G., Gani, R.
Publication date: 2012
Peer-reviewed: Yes
Electronic versions:
AIChE_Paper 246e.pdf
URLs:
https://aiche.confex.com/aiche/2012/webprogram/Paper278824.html

Bibliographical note
Oral presentation.
Source: dtu
Source-ID: u::4482
Research output: Research - peer-review › Article in proceedings – 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
Contributors: Mollerup, A. H., Mauricio Iglesias, M., Mikkelsen, P. S., Johansen, N. B., Thorberg, D., Sin, G.
Publication date: 2012

Event information
Event: 17th Nordic Process Control Workshop
Location: Kongens Lyngby, Denmark
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
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
Publication date: 2012

**Host publication information**

Title of host publication: Proceedings of IWA Nutrient Removal and Recovery 2012 : Trends in NRR
Keywords: Modeling, Autotrophic nitrogen removal, Anammox, Parameter estimation, Calibration and validation
Source: dtu
Source-ID: u::5175
Research output: Research - peer-review › Article in proceedings – Annual report year: 2012

**Event information**

Event: IWA Nutrient Removal and Recovery 2012
Location: Harbin, China

Calibration and validation of model describing complete autotrophic nitrogen removal in granular sludge

**General information**

State: Published
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Publication date: 2012

**Host publication information**

Title of host publication: Proceedings of IWA Nutrient Removal and Recovery 2012 : Trends in NRR
Keywords: Modeling, Autotrophic nitrogen removal, Anammox, Parameter estimation, Calibration and validation
Source: dtu
Source-ID: u::5175
Research output: Research - peer-review › Article in proceedings – Annual report year: 2012

**Event information**

Event: IWA Nutrient Removal and Recovery 2012
Location: Harbin, China

Controller tuning in wastewater treatment plants

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Mauricio Iglesias, M., Jørgensen, S. B., Sin, G.
Publication date: 2012

**Event information**

Event: 8th IFAC Symposium on Advanced Control of Chemical Processes
Location: Singapore, Singapore
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 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
Contributors: Abdul Samad, N. A. F. B., Gani, R., Gernaey, K., Sin, G.
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Publication date: 2012

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Bibliographical Note

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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...
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

the disturbances before the Anammox reactor.
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
Contributors: Hukkerikar, A., Jones, M. N., Sin, G., Gani, R.
Number of pages: 1
Publication date: 2012
Peer-reviewed: No
Event: Abstract from 18th Symposium on Thermophysical Properties, Boulder, CO, United States.
Electronic versions: AMH_ThermoSymposium_Abstract_2.pdf

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Oral presentation.
Source: dtu
Source-ID: u::4460
Research output: Research › Conference abstract for conference – Annual report year: 2012

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

Energibesparende biologisk proces til kvælstoffjernelse i spildevand

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Department of Environmental Engineering, Environmental Chemistry
Pages: 16-18
Publication date: 2012
Peer-reviewed: Yes

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Issue number: 10
ISSN (Print): 0011-6335
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ISI indexed (2013): ISI indexed no
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ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Electronic versions: PEC12-45.pdf
Source: dtu
Source-ID: u::5168
Research output: Research - peer-review › Journal article – Annual report year: 2012
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, poly functional 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), 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.

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, Chulalongkorn University
Contributors: Hukkerikar, A., Kalakul, S., Sarup, B., Young, D. M., Sin, G., Gani, R.
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Peer-reviewed: Yes

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Journal: Journal of Chemical Information and Modeling
Volume: 52
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  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 1
  Scopus rating (2017): CiteScore 3.9 SJR 1.349 SNIP 1.206
  Web of Science (2017): Impact factor 3.804
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): CiteScore 3.84 SJR 1.474 SNIP 1.193
  Web of Science (2016): Impact factor 3.76
  BFI (2015): BFI-level 1
  Scopus rating (2015): CiteScore 4.27 SJR 1.575 SNIP 1.281
  BFI (2014): BFI-level 1
  Scopus rating (2014): CiteScore 3.88 SJR 1.433 SNIP 1.244
  Web of Science (2014): Impact factor 3.738
  BFI (2013): BFI-level 1
  Scopus rating (2013): CiteScore 4.4 SJR 1.654 SNIP 1.334
  Web of Science (2013): Impact factor 4.068
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 1
  Scopus rating (2012): CiteScore 4.22 SJR 1.518 SNIP 1.342
  Web of Science (2012): Impact factor 4.304
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 1
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 property modeling and uncertainty analysis. 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.
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, Alfa Laval Copenhagen A/S
Contributors: Hukkerikar, A., Sarup, B., Abildskov, J., Sin, G., Gani, R.
Number of pages: 1
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Event: Abstract from 18th Symposium on Thermophysical Properties, Boulder, CO, United States.
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Bibliographical note
Oral presentation
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Source-ID: u::4459
Research output: Research › Conference abstract for conference – 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 Maritime
Contributors: Komulainen, T. M., Enemark-rasmussen, R., Sin, G., Fletcher, J. P., Cameron, D.
Pages: e153-e162
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Journal: Education for Chemical Engineers
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.98 SJR 0.273 SNIP 1.092
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.97 SJR 0.388 SNIP 0.686
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.75 SJR 0.303 SNIP 0.709
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.85 SJR 0.367 SNIP 0.947
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.69 SJR 0.261 SNIP 0.504
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.42 SJR 0.726 SNIP 1.784
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.47 SJR 0.253 SNIP 0.85
ISI indexed (2011): ISI indexed no
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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Mitrofanov, I., Abildskov, J., Sin, G., Gani, R.
Publication date: 2012
Peer-reviewed: No
Event: Abstract from CHISA 2012, Prague, Czech Republic.
Electronic versions:
IGM_CHISA2012_oral_abstract.pdf

Bibliographical note
Oral presentation.
Source: dtu
Source-ID: u::5180
Research output: Research › Conference abstract for conference – Annual report year: 2012

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
Contributors: Hukkerikar, A., Sarup, B., Young, D., Sin, G., Gani, R.
Number of pages: 2
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Electronic versions:
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URLs:
https://aiche.confex.com/aiche/2012/webprogram/Paper262554.html

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Oral presentation.
Source: dtu
Source-ID: u::5312
Research output: Research › Conference abstract for conference – Annual report year: 2012

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.
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
Contributors: Mauricio Iglesias, M., Valverde Perez, B., Sin, G.
Number of pages: 6
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Incremental design of control system of SHARON-Anammox process for autotrophic nitrogen removal

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Mauricio Iglesias, M., Valverde Perez, B., Sin, G.
Publication date: 2012

Event information
Event: 10th European Workshop on Advanced Control and Diagnosis
Location: Technical University of Denmark, Kgs. Lyngby, Denmark

Bibliographical note
Oral presentation.
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Source-ID: u::5416
Research output: Research › Sound/Visual production (digital) – 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
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
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Volume: 38
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
Web of Science (2017): Impact factor 3.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1 SNIP 1.631
Web of Science (2016): Impact factor 3.024
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.713
Web of Science (2015): Impact factor 2.581
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.22 SJR 1.168 SNIP 1.728
Web of Science (2014): Impact factor 2.784
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.06 SJR 1.21 SNIP 1.744
Web of Science (2013): Impact factor 2.452
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.05 SJR 1.138 SNIP 1.897
Web of Science (2012): Impact factor 2.091
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.8 SJR 1.44 SNIP 1.736
Web of Science (2011): Impact factor 2.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.167 SNIP 1.752
Web of Science (2010): Impact factor 2.072
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.171 SNIP 2.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.288 SNIP 2.094
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.621 SNIP 1.916
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.306 SNIP 1.888
Scopus rating (2005): SJR 1.306 SNIP 1.882
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.112 SNIP 1.86
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.332 SNIP 1.884
Scopus rating (2002): SJR 0.8 SNIP 0.916
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.951 SNIP 0.745
Web of Science (2001): Indexed yes
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.

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.
Molecular structure based physical properties modelling

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Cunico, L., Hukkerikar, A., Sin, G., Gani, R.
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Peer-reviewed: No
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Research output: Research › Conference abstract for conference – Annual report year: 2012

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 multi-enzyme 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 development process 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. Multi-enzyme 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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
pH variation and influence in an autotrophic nitrogen removing biofilm system: An efficient numerical solution strategy

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Vangsgaard, A. K., Mauricio Iglesias, M., Valverde Perez, B., Gernaey, K., Sin, G.
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Research output: Research - peer-review › Poster – Annual report year: 2012

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
Contributors: Vangsgaard, A. K., Mauricio Iglesias, M., Valverde Perez, B., Gernaey, K., Sin, G.
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Research output: Research - peer-review › Article in proceedings – Annual report year: 2012

Proceedings of the 17th Nordic Process Control Workshop

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Number of pages: 208
Publication date: 2012
Quantifying uncertainties of nucleation and crystal growth models on PAT system performance for crystallization processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Contributors: Abdul Samad, N. A. F. B., Meisler, K. T., Sin, G., Gernaey, K., Gani, R.
Number of pages: 1
Publication date: 2012
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Research output: Research › Conference abstract for conference – Annual report year: 2012

Recent trends in modelling and simulation of biological nutrient removal systems

General information
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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, Autonomous University of Barcelona
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Recent trends in modelling and simulation of nutrient removal systems

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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, Autonomous University of Barcelona
Pages: 29-32
Publication date: 2012

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Title of host publication: Proceedings of IWA Nutrient Removal and Recovery 2012: Trends in NRR
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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 firstorder 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
Contributors: Ramin, E., Flores-Alsina, X., Sin, G., Gernaey, K., Jeppsson, U., Mikkelsen, P. S., Plósz, B.
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Publisher: International Environmental Modelling and Software Society, iEMSs
Keywords: Modelling, ASM, BSM, Water quality, Simulators, Uncertainty, Good modelling practice, Sensitivity analysis
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Source: dtu
Source-ID: u::4431

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
Contributors: Castro, I. M., Mauricio Iglesias, M., Mollerup, A. L., Sin, G.
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Event information
Event: 11th IWA conference on instrumentation control and automation
Location: Narbonne, France
Research output: Research - peer-review › Article in proceedings – Annual report year: 2012

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.
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.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CAPEC-PROCESS, Alfa Laval Copenhagen A/S
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Publication date: 2012

Host publication information

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Publisher: Elsevier
Editors: Karimi, I., Srinivasan, R.
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Electronic versions:
AMH_MJ_BS_JA_GSI_RaG_PSE2012_abstract.pdf
Source: dtu
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Research output: Research - peer-review › Article in proceedings – Annual report year: 2012

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 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.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Computer Aided Process Engineering Center
Contributors: Jones, M. N., Hukkerikar, A., Sin, G., Gani, R.
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Event: Abstract from CHISA 2012, Prague, Czech Republic.
Electronic versions:
Mark Jones_AMH_GSI_RaG_CHISA2012_oral abstract.pdf

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Oral presentation.
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Source-ID: u::5178
Research output: Research › Conference abstract for conference – Annual report year: 2012

Separation of azeotropic mixtures

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
Contributors: Fernández, E., Gani, R., Sin, G.
Publication date: 2012
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Event: Abstract from ANQUE ICCE 2012, Sevilla, Spain.

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Research output: Research › Conference abstract for conference – Annual report year: 2012

Solventpro: The Solvent Selection and Design Framework

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Mitrofanov, I., Sin, G., Gani, R.
Publication date: 2012
Peer-reviewed: Yes
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
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
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
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(Key Computer Aided Chemical Engineering, Vol. 30).
Keywords: 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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Contributors: Quaglia, A., Sin, G., Gani, R., Sarup, B.
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Electronic versions:
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Oral presentation.
Source: dtu
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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
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
Number of pages: 2
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General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
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Research output: Research - peer-review › Poster – Annual report year: 2012

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.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Firmenich Inc.
Contributors: Heitzig, M., Rong, Y., Gregson, C., Sin, G., Gani, R.
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Publication information
Journal: Chemical Engineering and Technology
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.36 SJR 0.493 SNIP 0.797
Web of Science (2017): Impact factor 1.588
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.47 SJR 0.527 SNIP 0.892
Web of Science (2016): Impact factor 2.051
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.57 SJR 0.606 SNIP 0.907
Web of Science (2015): Impact factor 2.385
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
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
State: Published
The Solvent Selection framework: solvents for organic synthesis, separation processes and ionic-liquids solvents

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.

Model-Based Integrated Process Design and Controller Design of Chemical Processes

This thesis describes the development and application of a new systematic model-based methodology for performing integrated process design and controller design (IPDC) of chemical processes. The new methodology is simple to apply, easy to visualize and efficient to solve. Here, the IPDC problem that is typically formulated as a mathematical programming (optimization with constraints) problem is solved by the so-called reverse approach by decomposing it into...
A biochemically structured model for ethanol fermentation by Kluyveromyces marxianus: A batch fermentation and kinetic study

Anaerobic batch fermentations of ricotta cheese whey (i.e. containing lactose) were performed under different operating conditions. Ethanol concentrations of ca. 22gL−1 were found from whey containing ca. 44gL−1 lactose, which corresponded to up to 95% of the theoretical ethanol yield within 15h. The experimental data could be explained by means of a simple knowledge-driven biochemically structured model that was built on bioenergetics principles applied to the metabolic pathways through which lactose is converted into major products. Use of the model showed that the observed concentrations of ethanol, lactose, biomass and glycerol during batch fermentation could be described within a ca. 6% deviation, as could the yield coefficients for biomass and ethanol produced on lactose. The model structure confirmed that the thermodynamics considerations on the stoichiometry of the system constrain the metabolic coefficients within a physically meaningful range thereby providing valuable and reliable insight into fermentation processes.

General information
State: Published
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Contributors: Sansonetti, S., Hobley, T. J., Calabrò, V., Villadsen, J., Sin, G.
A framework for model-based optimization of bioprocesses under uncertainty: Identifying critical parameters and operating variables

This study presents the development and application of a systematic model-based framework for bioprocess optimization, evaluated on a cellulosic ethanol production case study. The implementation of the framework involves the use of dynamic simulations, sophisticated uncertainty analysis (Monte-Carlo technique) and sensitivity analysis (such as global techniques). The results of the case study point towards the enzyme loading as the most significant variable influencing the operational cost of additives in the conversion of lignocellulose to ethanol. Moreover, the results also show that there is an opportunity for further process optimization of bioethanol production from lignocellulose.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Meyer, A. S., Gernaey, K., Sin, G.
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A Framework for Optimization of Bioprocess Operation under Uncertainties: A lignocellulosic Ethanol Production Case Study

General information
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prod21320325610134.RMR_AIChE_Poster[1].pdf

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Research output: Research - peer-review › Poster – Annual report year: 2011

A generic multi-dimensional model-based system for batch cooling crystallization processes
Highly porous deposits of flame-made aerosol nanoparticles were formed by filtration through a porous substrate (α-alumina, average pore diameter 3.7 μm). The aerosol was characterized by transmission electron microscopy (TEM) and scanning mobility particle sizer (SMPS) showing average primary and agglomerate particle sizes of 4.1 and 30 nm, respectively. The analysis of the cake structure (determination of pore-size, dec, and porosity, εc) was carried out by two non-destructive permeance methods. The first (“method I”) was based solely on the dusty gas model (DGM) for mass-transfer. Thereafter, an expression (“method II”) for the calculation of the cake porosity was derived for Knudsen numbers N10. Permeance analysis revealed poresize (equivalent cylindrical diameter) of the deposited cakes of approximately 200 nm, independent of mass deposited (wd=0.7–36.8 mg). Calculation of the porosity by method I was prone to large errors due to any anisotropy of the porosity and resulted in unrealistically high εc values at low deposited mass (e.g. εc=0.99 at wd=0.7 mg). In contrast, the porosities (average εc=0.947–0.949) calculated by method II were independent of deposited mass and in excellent agreement to scanning electron microscopy (SEM) analysis (εc=0.94–0.97), as well as to previous studies at comparable experimental conditions (εc=0.95).

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abdul Sarnad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
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Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
Web of Science (2017): Impact factor 3.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1 SNIP 1.631
Web of Science (2016): Impact factor 3.024
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.713
Web of Science (2015): Impact factor 2.581
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.22 SJR 1.168 SNIP 1.728
Web of Science (2014): Impact factor 2.784
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.06 SJR 1.21 SNIP 1.744
Web of Science (2013): Impact factor 2.452
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.05 SJR 1.138 SNIP 1.897
Web of Science (2012): Impact factor 2.091
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.8 SJR 1.144 SNIP 1.736
Web of Science (2011): Impact factor 2.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.167 SNIP 1.752
Web of Science (2010): Impact factor 2.072
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.171 SNIP 2.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.288 SNIP 2.094
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.621 SNIP 1.916
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.306 SNIP 1.888
Scopus rating (2005): SJR 1.306 SNIP 1.882
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.112 SNIP 1.86
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.332 SNIP 1.884
Scopus rating (2002): SJR 0.8 SNIP 0.916
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.951 SNIP 0.745
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.125 SNIP 1.054
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.05 SNIP 1.131
Original language: English
A Mathematical Model for Simultaneous Saccharification and Co-fermentation (SSCF) of C6 and C5 Sugars

Reliable production of biofuels and specifically bioethanol has attracted a significant amount of research recently. Within this context, this study deals with dynamic simulation of bioethanol production processes and in particular aims at developing a mathematical model for describing simultaneous saccharification and co-fermentation (SSCF) of C6 and C5 sugars. The model is constructed by combining existing mathematical models for enzymatic hydrolysis and co-fermentation. An inhibition of ethanol on cellulose conversion is introduced in order to increase the reliability. The mathematical model for the SSCF is verified by comparing the model predictions with experimental data obtained from the ethanol production based on kraft paper mill sludge. When fitting the model to the data, only the yield coefficients for glucose and xylose metabolism were fine-tuned, which were found to be 0.43 g·g⁻¹ (ethanol/glucose) and 0.35 g·g⁻¹ (ethanol/xylose) respectively. These promising validation results encourage further model application to evaluate different process configurations for lignocellulosic bioethanol technology.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.37 SJR 0.403 SNIP 0.76
Web of Science (2016): Impact factor 1.174
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.61 SJR 0.5 SNIP 1.111
Web of Science (2015): Impact factor 1.207
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.53 SJR 0.56 SNIP 1.175
Web of Science (2014): Impact factor 1.098
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.4 SJR 0.514 SNIP 1.204
Web of Science (2013): Impact factor 0.872
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.29 SJR 0.543 SNIP 1.121
Web of Science (2012): Impact factor 0.92
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
An integral analysis for second generation bioethanol production via a dynamic model-based simulation approach: stochastic nonlinear optimisation

There are different technological routes to biofuels production such as, biohydrogen, biomethane, biobutanol, among others. Bioethanol production from lignocellulosic feedstock has acquired special attention, and its feasibility has been demonstrated at laboratory, pilot and demo-plant scale[1,2,3]. Despite the reported progress and the promising results, however, at present this technology is not cost-competitive compared with first generation bioethanol production or fossil-fuels. Therefore, there is further room for optimisation of the technology and improvement of its cost-effectiveness. The objective of this study is to perform an integral analysis for bioethanol production from lignocellulosic feedstock using a rigorous dynamic modelling approach for the whole process. The bioethanol production includes different sections such as, pre-treatment of the substrate, enzymatic hydrolysis of cellulose, co-fermentation of sugars and downstream processes for purification and recovery of most value-added products. The dynamic model involves both the mass and energy balances coupled with constitutive dynamic equations to assess the process yield and energy efficiency of different bioethanol processes. This study employs the Dynamic Lignocellulosic Bioethanol (DLB 1.0) modelling platform[4], which has demonstrated to describe accurately the dynamics of the pre-treatment, enzymatic hydrolysis and co-fermentation. Moreover, DLB 1.0 is complemented by downstream process models. The results will show and provide further analysis for 2G bioethanol production, aiming to decrease and find a competitive bioethanol production cost that recently was set on $2.35 USD/gallon[5]. Thus, the application of the constructed modelling platform will allow and support the analysis and search of a more reliable and feasible bioethanol production route.
Application of computer-aided multi-scale modelling framework - Aerosol case study

A computer-aided modelling tool for efficient multi-scale modelling has been developed and is applied to solve a multi-scale modelling problem related to design and evaluation of fragrance aerosol products. The developed modelling scenario spans three length scales and describes how droplets of different sizes are formed when a liquid fragrance product is sprayed from a pressurized can and how these droplets evaporate while they settle down due to sedimentation and convective mixing.

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Source: orbit
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Research output: Research - peer-review › Article in proceedings – Annual report year: 2011

Application of computer-aided multi-scale modelling framework – Aerosol case study

Model-based computer aided product-process engineering has attained increased importance in a number of industries, including pharmaceuticals, petrochemicals, fine chemicals, polymers, biotechnology, food, energy and water. This trend is set to continue due to the substantial benefits computer-aided methods provide. The key prerequisite of computer-aided product-process engineering is however the availability of models of different types, forms and application modes. The development of the models required for the systems under investigation tends to be a challenging and time-consuming task involving numerous steps, expert skills and different modelling tools. This motivates the development of a computer-aided modelling framework that supports the user during model development, documentation, analysis, identification, application and re-use with the goal to increase the efficiency of the modelling process. The developed modelling framework is structured based on the work-flow and data-flow the modeller needs to follow to fulfil the desired modelling task. The framework consists of two main parts (work-flows) for model development. The first part is dedicated to single-scale model development while the second part supports the modeller during the multi-scale scenario development and comparison. The second part of the modelling framework manages different multi-scale scenarios, supports in the systematic derivation of a new scenario and links the models for the different scales according to the linking scheme of the multi-scale scenario. This is where the single-scale model development part is connected to the multi-scale scenario development part because it assists the modeller in providing the single-scale models that are being linked to form the multi-scale scenario. The single-scale model development part supports the modeller in model documentation, construction and analysis. Different models for properties, phenomena, unit operations, processes can be developed and analysed here or retrieved from model libraries. The model equations are introduced in a simple text format and are translated by the modelling tool with the reverse polish notation (RPN). A model object is generated which can be applied in a stand-alone mode, stored in libraries and/or linked to other models. The model analysis section contains different eigenvalue analysis. Once the models have been constructed and analysed the modelling framework incorporates 3 application work-flows: identification, simulation and design. For these application work-flows different solvers that can solve a large range of different problems are connected to the modelling tool. The tool is able to determine the solution strategy together with the required solvers based on the results of the model analysis during model development. For model identification features like sensitivity analysis, identifiability analysis, optimizer, confidence interval calculation and uncertainty analysis have been incorporated into the tool. The structure of the modelling tool as well as its features will be highlighted through a case study involving a problem from industry related to multi-scale model development and application.
Application of the Morris method for screening the influential parameters of fuzzy controllers applied to WWTPs

In this paper, we evaluate the application of a sensitivity analysis to help fine-tuning a fuzzy controller for a biological nitrogen and phosphorus removal (BNPR) plant. The Morris Screening method is proposed and evaluated as a prior step to obtain the parameter significance ranking. First, an iterative procedure has been performed in order to find out the proper repetition number of the elementary effects (r) of the method. The optimal repetition number found in this study (r = 60) is in direct contrast to previous applications of the Morris method, which usually use low repetition number, e.g. r = 10 - 20. Working with a non-proper repetition number (r) could lead to Type I error (identifying a not-important factor as significant (false positive)) as well as Type II error (identifying an important factor as not significant (false negative)), hence emphasizing the importance of finding the optimal repetition number for each study in question. With the proper r found, the Morris Screening helped identify the parameter significance ranking, thereby facilitating the calibration of fuzzy controllers, which contain many parameters that need to be adjusted for different wastewater treatment plant (WWTP) applications.
Although being a mature and well established industry segment, over the last few decades the vegetable oil industry has been facing many important new challenges due to emerging new products (such as biodiesel and nutraceuticals compounds), as well as new trends and regulations with regards to sustainability, environment and health. Most of the time, the industry reacted to these challenges taking decisions based on previous experiences or heuristic, or with the help of tools which arguably were not fit to manage the complexity of the entire value chain, and therefore often led to suboptimal outcomes. In this paper, a systematic framework for Computer-Aided Flowsheet Syntesis and Design (CAFD)
and resources allocation for the vegetable oil sector is presented. In the framework a Mixed Integer Non Linear Programming (MINLP) problem is formulated and solved for a soybean processing case study, to determine the optimal processing network for vegetable oil extraction and refining (including biodiesel production and various options for byproducts valorization), as well as the optimal material flows to each processing step. In order to optimize the resources needed to solve such a large and complex problem, an efficient and systematic solution strategy based on the use of shortcut calculations to eliminate infeasible and redundant options to reduce the search space for the rigorous optimization problem is adopted. One of the main advantages of the use of this framework is its ability to generate different scenarios by changing the input data, without having to modify the model structure. Also, the framework can be adapted to different purposes, from retrofit of existing operations to new plant design, by changing variable specifications.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
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Event: Abstract from 8th European Congress of Chemical Engineering, Berlin, Germany.
Source: orbit
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A Systematic Methodology for the Assessment and Troubleshooting of Control Strategies and Operational Problems In Distillation Systems

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, NNE Pharmaplan
Contributors: Mauricio Iglesias, M., Johansen, K., Jørgensen, S. B., Sin, G.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 2011 AIChE Annual Meeting, Minneapolis, MN, United States.
Electronic versions:
prod21320326700534.MMI_AiChe_abstract[1].pdf
URLs:
Source: orbit
Source-ID: 312252
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

A Systematic Methodology for Uncertainty Analysis of Group Contribution Based and Atom Connectivity Index Based Models for Estimation of Properties of Pure Components

One of the most widely employed group contribution method for estimation of properties of pure components is the Marrero and Gani (MG) method. For the given component whose molecular structure is not completely described by any of the available groups, group contribution+ method (combined MG method and atomic connectivity index method) has been employed to create the missing groups and predict their contributions through the regressed contributions of connectivity indices. The objective of this work is to develop a systematic methodology to carry out uncertainty analysis of group contribution based and atom connectivity index based property prediction models. This includes: (i) parameter estimation using available MG based property prediction models and large training sets to determine improved group and atom contributions; and (ii) uncertainty analysis to establish statistical information such as covariance, standard error and confidence intervals. The developed methodology allows estimation of following properties: normal boiling point, critical constants, standard enthalpy of formation, standard enthalpy of vaporization, standard Gibbs energy, normal melting point, standard enthalpy of fusion, entropy of vaporization, surface tension, viscosity, flash point, auto ignition temperature, Hansen solubility parameters, Hildebrand solubility parameter, aqueous solubility, octanol/water partition coefficient, compressibility factor, molar volume, molar refraction, refractive index and lethal concentration. The application of the developed methodology is highlighted through a set of molecules not used in the parameter estimation step. The developed methodology can be used to assist uncertainty and sensitivity analysis of product/process design to obtain rationally the risk/ safety factors and to provide confidence in the obtained process calculations.

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State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
Building a multilevel modeling network for lipid processing systems

The aim of this work is to present the development of a computer-aided multilevel modeling network for the systematic design and analysis of processes employing lipid technologies. This is achieved by decomposing the problem into four levels of modeling: i) pure component property modeling and a lipid-database of collected experimental data from industry and generated data from validated predictive property models, as well as modeling tools for fast adoption-analysis of property prediction models; ii) modeling of phase behavior of relevant lipid mixtures using the UNIFAC-CI model, development of a master parameter table and calculations of the activity coefficients (VLE) related to a multicomponent system; iii) development of a model library consisting of new and adopted process models of unit operations involved in lipid processing technologies, validation of the developed models using operating data collected from existing process plants, and application of validated models in design and analysis of unit operations; iv) the information and models developed are used as building blocks in the development of methods and tools for computer-aided synthesis and design of process flowsheets (CAFD). The applicability of this methodology is highlighted in each level of modeling through the analysis of a lipid process that has significant relevance in the edible oil and biodiesel industries since it determines the quality of the final oil product, the physical refining process of oils and fats.

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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, Alfa Laval Copenhagen A/S
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Publication date: 2011

Building a Multilevel Modeling Network for Lipid Processing Systems

The world’s fats and oils production has been growing rapidly over the past few decades, exceeding the need for human nutrition. This overproduction combined with the increasing interest among the consumers for healthier food products and bio-fuels, has led the oleo chemical industry to face in the upcoming years major challenges in terms of design and development of better products and more sustainable processes. Although the oleo chemical industry is mature and based on well established processes, the complex systems that lipid compounds form, the lack of accurate predictive models for their physical properties and unit operation models for their processing have limited computer-aided methods and tools for process synthesis, modeling and simulation to be widely used for design, analysis, and optimization of these processes.

The world’s fats and oils production has been growing rapidly over the past few decades, exceeding the need for human nutrition. This overproduction combined with the increasing interest among the consumers for healthier food products and bio-fuels, has led the oleo chemical industry to face in the upcoming years major challenges in terms of design and development of better products and more sustainable processes. Although the oleo chemical industry is mature and based on well established processes, the complex systems that lipid compounds form, the lack of accurate predictive models for their physical properties and unit operation models for their processing have limited computer-aided methods and tools for process synthesis, modeling and simulation to be widely used for design, analysis, and optimization of these processes.

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Computer Aided Flowsheet Synthesis and Design Under Uncertainty In Vegetable Oil Production

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
Contributors: Quaglia, A., Sarup, B., Sin, G., Gani, R.
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Computer-aided modeling for efficient and innovative product-process engineering

Model-based computer aided product-process engineering has attained increased importance in a number of industries, including pharmaceuticals, Petrochemicals, fine chemicals, polymers, biotechnology, food, energy and water. This trend is set to continue due to the substantial benefits computer-aided methods provide. The key prerequisite of computer-aided product-process engineering is however the availability of models of different types, forms and application modes. The development of the models required for the systems under investigation tends to be a challenging, time-consuming and therefore cost-intensive task involving numerous steps, expert skills and different modelling tools. The objective of this project is to systematize the process of model development and application thereby increasing the efficiency of the modeller as well as model quality.

The main contributions of this thesis are a generic methodology for the process of model development and application, combining in-depth algorithmic work-flows for the different modelling tasks involved and the development of a computer-aided modelling framework. This framework is structured, is based on the generic modelling methodology, partially automates the involved work-flows by integrating the required tools and, supports and guides the user through the different work-flow steps. Supported modelling tasks are the establishment of the modelling objective, the collection of the required system information, model construction including numerical analysis, derivation of solution strategy and connection to appropriate solvers, model identification/discrimination as well as model application for simulation and optimization. The computer-aided modelling framework has been implemented into a userfriendly software.

A variety of case studies from different areas in chemical and biochemical engineering have been solved to illustrate the application of the generic modelling methodology, the computer-aided modelling framework and the developed software tool.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Gani, R., Sin, G., Glarborg, P.
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Computer-aided modeling framework for efficient model development, analysis and identification: Combustion and reactor modeling

Model-based computer aided product-process engineering has attained increased importance in a number of industries, including pharmaceuticals, petrochemicals, fine chemicals, polymers, biotechnology, food, energy, and water. This trend is set to continue due to the substantial benefits computer-aided methods introduce. The key prerequisite of computer-aided product-process engineering is however the availability of models of different types, forms, and application modes. The development of the models required for the systems under investigation tends to be a challenging and time-consuming task involving numerous steps, expert skills, and different modeling tools. This paper introduces a generic methodology that structures the process of model development, analysis, identification, and application by providing the modeler with the work-flow that needs to be followed in a systematic manner. The methodology has been implemented into a computer-aided modeling framework, which combines expert skills, tools, and database connections that are required for the different steps of the model development work-flow with the goal to increase the efficiency of the modeling process. The framework has two main branches; the first branch deals with single-scale model development while the second branch introduces features for multiscale model development to the methodology. In this paper, the emphasis is on single-scale model development and application part. The modeling framework and the supported stepwise model development is highlighted through a case study related to air pollution control, namely, the thermal treatment of the off-gas stream in adipic acid production in order to reduce its N2O content.

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Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
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Computer Aided Solvent Selection and Design Framework

Solvents are widely used as a reaction medium, as a reactant or as carrier at some stages of the manufacturing chain in products from the chemical, fine chemical, pharmaceutical, food, and agrochemical industries. Solvent are either required for processing after which they are removed or they are part of the final product formulation. Therefore, solvents are playing an important role in product synthesis and formulation, product delivery, separation processes etc [1]. On the other hand, solvent selection and design is a complex problem, which requires decision making in several levels for indentifying the best candidates depending on different multi-objective criteria namely environment, health, safety, process feasibility and economics. One of the criteria of solvent selection is the environmental impact because of the excessive consumption...
and utilization in a wide range of industries, millions of tons solvents have to be wasted every year [2]. Therefore, it becomes important to minimize and optimize the use of organic solvents as much as possible, to satisfy the “Green Chemistry Principles” [3]. Another challenge is that currently solvent selection relies very much on previous experiences, trial and error with different solvent candidates. Such heuristic approach while valuable on their own, however arguably are not fit to deal with a complex multi-criteria optimization and search problem, which is the case for solvent selection. Therefore the purpose of this contribution is to develop a systematic framework and implement it as software for selection and design of solvents for many applications including organic synthesis, complex reaction systems and solvent-based separations. The solvent selection framework is based on a combination of knowledge from industrial practice and computer-aided tools and methods for property prediction and computer-aided molecular design (CAMD) principles. This framework is applicable for solvent selection and design in product design as well as process design. The first module of the framework is dedicated to the solvent selection and design for organic synthesis. This part uses the solvent selection methodology of Gani et al. [4,5], which has been extended to handle multi-step chemical syntheses as well as solvent substitution for specific reaction steps in existing processes. The methodology for organic synthesis accordingly involves five steps for each reaction: 1. Problem identification. Finding an objective for given system, identifying actual functions of the solvent. 2. Search criteria definition. The solvent functions that satisfy the operational needs of the process are defined in terms of a set of search criteria (R-indices), defined in terms of: physical and chemical properties (solvent–pure properties); Environment, Health and Safety (EHS) characteristic (solvent–EHS properties); operational properties (solvent–solute properties). 3. Performing the search. The search step consists of two stages. The first is a generation and property identification of solvent candidates using special software ProCAMD and ProPred, which are the implementations of computer-aided molecular techniques. The second consists of assigning the RS-indices following the reaction–solvent and then consulting the known solvent database and identifying the set of solvents that satisfy search criteria. 4. Score table assignment. A list of feasible solvents needs to be created. The scores are assigned from the calculated values of RS indices. The scores give a weight to each of the calculated RS indices. 5. Matrix of solvents. After the scores table has been generated, a short list of feasible solvents is obtained for each reaction step. This methodology has been evaluated with several practical application examples including a single reaction solvent screening problem, a solvent replacement problem and a solvent selection for a multi-stage system. The second module of the framework is dedicated to solvent selection for separation processes. One of the important tasks in separation processes is an identification of a pure solvent or anti-solvent for a specific Active Pharmaceutical Ingredient, which is a problem of major concern for the pharmaceutical R&D departments. Solvents, lipids and other compounds are commonly employed in product formulation as well as in APIs processing. In addition, the design of solvent mixtures that sometimes show improved characteristics of solubility toward a particular API could bring several advantages. The framework includes a model-based method for solvent screening and solvent mixtures design for pharmaceutical applications. The problems that can be solved with this method are the following: given an API, select a good solvent or a good antisolvent; design a solvent mixture that improves the solubility if the solubility target cannot be reached with a single solvent; identify the optimal antisolvent that added in mall amount to the mixture API-solvent gives the highest precipitation of API (for crystallization processes). The method is based on the theory of the conceptual segments (hydrophobic, polar and hydrophilic) introduced by Chau-Chyun and Song (2004) with the NRTL-SAC method [6]. In order to make the method completely independent from the availability of experimental data, a Marrero and Gani (2001) Group Contribution model (M&G GC+) [7] is for the prediction of the conceptual segments is developed in this work. With the above model, the API molecule can be described in terms of conceptual segments (first step of the method) and, then, the solvent power of the pure solvents can be computed and ranked from the best to the worst (anti-solvent). Hence, the design of a solvent mixture that enhances the API solubility can be performed by identifying the conceptual segments combination that maximizes the excess properties. An anti-solvent that mixed with the best solvent gives a large decrease in the API solubility can be identified in the same way as before, but this time excess properties of mixing have to be minimized.
Development of Property Models with Uncertainty Estimate for Process Design under Uncertainty

Physical and thermodynamic properties of pure compounds and their mixtures play an important role in design, simulation and optimization of chemical processes. The accuracy of process design and simulation largely depends on the accuracy of the underlying physical and thermodynamic data and property prediction models. While use of experimentally measured values for the needed properties is desirable in process design, the experimental data for the compounds of interest may not be available in many cases. Therefore, development of efficient and reliable property prediction methods and tools that can also provide estimates of uncertainties in predictions of properties and their effects on process design becomes necessary. For instance, the accuracy of design of distillation column to achieve a given product purity is dependent on many pure compound properties such as critical pressure, critical temperature, acentric factor etc. In such cases, accurate property values along with uncertainty estimates are needed to perform sensitivity analysis and quantify the effects of these uncertainties on the process design. The objective of this work is to develop a systematic methodology to provide more reliable predictions with a new and improved set of model parameters for GC (group contribution) based and CI (atom connectivity index) based models and to quantify the uncertainties in the estimated property values from a process design point-of-view. This includes: (i) parameter estimation using available GC based and CI based property prediction models and large training sets to determine improved group and atom contributions; (ii) uncertainty analysis of property prediction models to establish statistical information such as covariance, standard error and confidence intervals; and (iii) use the results of uncertainty analysis to predict the uncertainties in process design. For parameter estimation, large datasets of experimentally measured property values for a wide range of pure compounds are taken from the CAPEC database. Classical frequentist approach i.e., least square method is adopted for the estimation of model prediction uncertainties. The developed methodology provides property values along with uncertainties for the following 20 properties: normal boiling point, critical temperature, critical pressure, critical volume, normal melting point, standard Gibbs energy, standard enthalpy of formation, standard enthalpy of fusion, standard enthalpy of vaporization at 298 K and at the normal boiling point, entropy of vaporization at the normal boiling point, surface tension at 298 K, viscosity at 300 K, flash point, auto ignition temperature, Hansen solubility parameters, Hildebrand solubility parameter, octanol/water partition coefficient, aqueous solubility, acentric factor, and liquid molar volume at 298 K. The performance of property models for these properties with the revised set of model parameters is highlighted through a set of compounds not considered in the regression step. The comparison of model prediction uncertainties with reported range of measurement uncertainties is presented for the properties with related available data. The application of the developed methodology to quantify the effect of these uncertainties on the design of different unit operations (distillation column, liquid-liquid extraction, heat exchanger, crystallizer, equilibrium reactor etc.) is presented. The results show that depending on the chemical systems involved and the operating conditions being considered, some of the input uncertainties can result in significant uncertainties in design. The most sensitive properties for each unit operation are also identified. This analysis can be used to reduce the uncertainties in property estimates for the properties of critical importance (by performing additional experiments to get better experimental data and better model parameter values). Thus, the developed methodology can be used to quantify the sensitivity of process design to uncertainties in property estimates; obtain rationally the risk/safety factors in process design; and identify additional experimentation needs in order to reduce most critical uncertainties.
In this study a number of different process flowsheets were generated and their feasibility evaluated using simulations of dynamic models. A dynamic modeling framework was used for the assessment of operational scenarios such as, fed-batch, continuous and continuous with recycle configurations. Each configuration was evaluated against the following benchmark criteria, yield (kg ethanol/kg dry-biomass), final product concentration and number of unit operations required in the different process configurations. The results show that simultaneous saccharification and co-fermentation (SSCF) operating in continuous mode with a recycle of the SSCF reactor effluent, results in the best productivity of bioethanol among the proposed process configurations, with a yield of 0.18 kg ethanol/kg dry-biomass.

**General information**

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
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Framework for Construction of Multi-scale Models for Biological Wastewater Treatment Processes

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Environmental Chemistry, Department of Environmental Engineering
Contributors: Vangsgaard, A. K., Mauricio Iglesias, M., Gernaey, K., Smets, B. F., Sin, G.
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Framework for Construction of Multi-scale Models for Biological Wastewater Treatment Processes - Case Study: Autotrophic Nitrogen Conversion

In wastewater treatment technologies, employing biofilms or granular biomass, processes might occur at very different spatial and temporal scales. Model development for such systems is typically a tedious, complicated, and time consuming task, which involves selecting appropriate model equations for the different scales, making appropriate and simplifying assumptions, connecting them through a defined linking scheme, analyzing and solving the model equations numerically, and performing parameter estimations if necessary. In this study, a structured framework for modeling such systems is developed. It aims to support the user at the various steps and to reduce the time it takes to generate a model ready for application. An implementation of the framework is illustrated using a simple case study, which considers treatment of a nitrogen-rich wastewater via nitritation.

Global sensitivity analysis in wastewater treatment plant model applications: Prioritizing sources of uncertainty

This study demonstrates the usefulness of global sensitivity analysis in wastewater treatment plant (WWTP) design to prioritize sources of uncertainty and quantify their impact on performance criteria. The study, which is performed with the Benchmark Simulation Model no. 1 plant design, complements a previous paper on input uncertainty characterisation and propagation (Sin et al., 2009). A sampling-based sensitivity analysis is conducted to compute standardized regression coefficients. It was found that this method is able to decompose satisfactorily the variance of plant performance criteria (with R2 > 0.9) for effluent concentrations, sludge production and energy demand. This high extent of linearity means that the plant performance criteria can be described as linear functions of the model inputs under the defined plant conditions. In effect, the system of coupled ordinary differential equations can be replaced by multivariate linear models, which can be used as surrogate models. The importance ranking based on the sensitivity measures demonstrates that the most influential factors involve ash content and influent inert particulate COD among others, largely responsible for the uncertainty in predicting sludge production and effluent ammonium concentration. While these results were in agreement with process knowledge, the added value is that the global sensitivity methods can quantify the contribution of the variance of significant parameters, e.g., ash content explains 70% of the variance in sludge production. Further the importance of formulating appropriate sensitivity analysis scenarios that match the purpose of the model application needs to be highlighted. Overall, the global sensitivity analysis proved a powerful tool for explaining and quantifying uncertainties as well as providing insight into devising useful ways for reducing uncertainties in the plant performance. This information can help engineers design robust WWTP plants.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.358
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Scopus rating (2016): CiteScore 7.49 SJR 2.663 SNIP 2.563
Web of Science (2016): Impact factor 6.942
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.63 SJR 2.665 SNIP 2.482
Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.13 SJR 2.946 SNIP 2.702
Web of Science (2014): Impact factor 5.528
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Scopus rating (2010): SJR 2.592 SNIP 2.192
Web of Science (2010): Impact factor 4.546
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BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.319 SNIP 2.224
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Scopus rating (2008): SJR 2.073 SNIP 2.178
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Web of Science (2005): Indexed yes
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Web of Science (2004): Indexed yes
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Integration of Generic Multi-dimensional Model and Operational Policies for Batch Cooling Crystallization

A generic multi-dimensional modeling framework for studying batch cooling crystallization processes under generated operational policies is presented. The generic nature of the modeling allows the study of a wide range of chemical systems under different operational scenarios, enabling thereby, the analysis of various crystallization operations and conditions. Furthermore, a systematic procedure for generating operational policies through available analytical crystal size distribution (CSD) estimators has been developed and verified for achieving targeted CSD consistently. The application of the model-based framework is highlighted for batch cooling crystallization of potassium dihydrogen phosphate (KDP) in two-dimensions, while the use of the analytical estimator is demonstrated for a potassium dichromate case study to achieve a target CSD.
Integration of Generic Multi-dimensional Model and Operational Policies for Batch Cooling Crystallization

Crystallization processes form an important class of separation methods that are frequently used in the chemical, the pharmaceutical and the food industry. The specifications of the crystal product are usually given in terms of crystal size, shape and purity. In order to predict the desired crystal morphology by means of model-based approaches, appropriate models covering the effects of the various operational parameters on the behavior of the crystals are necessary. Therefore the generic model-based framework of one dimension crystallization processes has been developed for process control and product monitoring to meet this need [1]. However the one-dimensional models only consider one inner variable (characteristic length) in the population balance equations as a measure for crystal size, thus limiting the crystal shape only to the description of spherical or cubic crystals. To fully characterize the crystal particles higher dimensional models are necessary, that is, a multi-dimensional population balance modeling approach is needed, where two- or even three-characteristic lengths of a crystal may be considered. Once the model is available, it can subsequently be used in many applications, notably to obtain the required product qualities in terms of CSD and shape. Usually the main difficulty in batch cooling crystallization is to accomplish a uniform and reproducible CSD. Usually supersaturation control has been applied to drive the process within the metastable zone to enhance the control of the CSD. Although this approach has shown to produce high quality crystals, the set point operating profiles for the supersaturation controller are usually chosen arbitrarily or by trial-and error. The objective of this work is to integrate generic multi-dimensional models with operational policies based on analytical estimators within a computer aided framework for study of batch cooling crystallization processes. Also, the paper highlights the application of the framework to study different multi-dimensional aspects of crystallization processes for a wide range of chemical systems. In order to generate an operational policy, an analytical CSD estimator has been introduced and integrated with the generic multi-dimensional model in the framework. The estimator is based on the assumptions of constant supersaturation and an operation that is dominated by size dependent growth. The generated operational policy provides the supersaturation set point and by maintaining the operation at this point, a target CSD is achieved. Compared to earlier works, additional information regarding the total crystal mass is also targeted here. The application of the multi-dimensional model-based framework is highlighted using a two-dimensional potassium dihydrogen phosphate (KDP) batch cooling crystallization process as a case study. The use of an analytical estimator for prediction of the CSD is illustrated on a potassium dichromate case study.

Lipid Processing Technology: Building a Multilevel Modeling Network

Over the past few decades, the world’s fats and oils production has been growing rapidly, far beyond the need for human nutrition. This overproduction combined with the growing consumer preferences for healthier food products and the interest in bio-fuels, has led the oleo chemical industry to face in the upcoming years major challenges in terms of design and development of better products and more sustainable processes. Although the oleo chemical industry is mature and based on well established processes, the complex systems that lipid compounds form, the lack of accurate predictive models for their physical properties and unit operation models for their processing have limited computer-aided methods and tools for process synthesis, modeling and simulation to be widely used for design, analysis, and optimization of these processes. In consequence, the aim of this work is to present the development of a computer aided multilevel modeling network consisting a collection of new and adopted models, methods and tools for the systematic design and analysis of processes employing lipid technology. This is achieved by decomposing the problem into four levels of modeling: 1. pure component properties; 2. mixtures and phase behavior; 3. unit operations; and 4. process synthesis and design. The methods and tools in each level include: For the first level, a lipid-database of collected experimental data from the open literature, confidential data from industry and generated data from validated predictive property models; as well as modeling tools for fast adoption. In the second level, phase behaviors (VLE, LLE and SLE) of relevant lipid mixtures are predicted using the UNIFAC-Ci model where missing group interaction parameters are predicted using the GCPlus approach (connectivity index). A master parameter table is prepared for this purpose. In the third level, a detailed computer aided model analysis of unit operations encountered in oleo chemical industry (e.g. Transesterification, Hydrogenation, Interesterification etc.), optimal design, operation and control of these unit operations with respect to performance parameters such as minimum total cost, product yield improvement, operability etc., and process intensification for the retrofit of existing biofuel plants. In the fourth level the information and models developed are used as building blocks in the development of methods and tools for computer-aided synthesis and design of process flowsheets (CAFD), feasibility assessment and comparison of the alternative flowsheets at their optimal operating points and optimization of the selected alternative with respect to cost and sustainability indicators.
Methodological Approach for Modeling of Multienzyme in-pot Processes

This paper presents a methodological approach for modeling multi-enzyme in-pot processes. The methodology is exemplified stepwise through the bi-enzymatic production of N-acetyl-D-neuraminic acid (Neu5Ac) from N-acetyl-D-glucosamine (GlcNAc). In this case study, sensitivity analysis is also used to evaluate the reliability of all parameters of the model suggested in literature [5]. Results, from the sensitivity analysis, are used as criteria for a systematic simplification of the model structure. Consequently, model complexity was reduced without compromising the general predictive performance. A deviation of less than 5% from the original model was found.

Micro2-Managed Microbial Communities: Next Generation Environmental Bio/Technologies

Microbes are amazingly diverse in terms of the reactions that they catalyze. This diversity can be exploited to create competitive biotechnological solutions for many environmental challenges, where the right combination of existing microbial reactions can convert unwanted pollutants into a useful or harmless end-product. There are, however, significant scientific and technical challenges in order to combine potentially useful microbial reactions into a workable biotechnology,
especially for processes that require the cooperation between microbial groups with very different properties and preferences. Simple empirical approaches often fail, and our intent is therefore to rationally manipulate the composition, that is, the microbial diversity of such systems, towards a target performance. Our hypothesis is that controlled biofilm or bioaggregate-based systems, wherein microbes grow in spatially structured assemblies, are suitable to harness these microbial potentials. We specifically aim to develop, implement and validate the feasibility of generic approaches for the rapid and efficient selection and management of the microbial composition and the micro-scale structure (micro2-management) of biofilms and bioaggregates for a target performance goal. These approaches are being implemented for the rapid start-up and high-rate operation of membrane-supported biofilm reactors and granular biomass reactors to attain a community consisting of aerobic and anaerobic ammonium oxidizing bacterial guilds (AeAOB and AnAOB) for autotrophic nitrogen (N) removal from wastewaters.

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**Modeling framework for multi-enzyme in-pot processes applied in amine production**

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Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011
Modelling and control of heat-integrated distillation columns: An industrial case study

Energy requirements of distillation processes account for a large percentage of the total energy consumption of the chemical industry. Hence, strategies for heat recovery have been extensively implemented in industrial processes during the last decades. However, operation (including start-up and shut-down strategies) and control of, heat-integrated systems becomes a formidable challenge if not a problem since higher-order systems dynamics occur where different time-scale phenomena interact. Furthermore, if the operation state of the process does not lie close to the designed state, the amount of energy wasted increases, questioning the economics of implementation of heat integration. Modelling is the foremost tool in assessment of chemical process dynamics. In the case of distillation, an extensive literature deals with classic distillation columns whereas much less has been investigated on dynamics of heat integrated distillation systems and the significance of developing a proper plantwide control strategy to ensure optimal and stable operation. This contribution has two aims; firstly to create a systematic framework for the modeler for developing dynamic models of distillation processes with heat-integration. To this end a computer-aided methodology was developed. Secondly, the methodology was tested in an actual industrial case, where a dynamic model for heat-integrated distillation systems is developed and used to analyse and solve operation and control problem. The system studied in the industrial case is composed of two distillation columns in series (operated at 3.5 and 1.5 bar) for recovery of ethanol from a pseudo-binary mixture (heavy key water). Heat recovery is carried out both backward (from the two bottoms flow to the feed) and forward (from the first condensate to the second reboiler). Based on a numerical model of the system, two solutions are presented for improving its control: i) a fine tuning of the existing control strategy, therefore suitable for immediate implementation; and ii) a new control structure, including sensors and actuators for long term modification of the system. The suitability of the proposed control strategies were ultimately evaluated using as input actual data of one month of operation.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, NNE Pharmaplan
Contributors: Mauricio Iglesias, M., Johansen, K., Jørgensen, S. B., Sin, G.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 8th European Congress of Chemical Engineering, Berlin, Germany.
Source: orbit
Source-ID: 312257
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Modelling Framework for the Identification of Critical Variables and Parameters under Uncertainty in the Bioethanol Production from Lignocellulose

This study presents the development of a systematic modelling framework for identification of the most critical variables and parameters under uncertainty, evaluated on a lignocellulosic ethanol production case study. The systematic framework starts with: (1) definition of the objectives; (2) Collection of data and the implementation of dynamic models for each unit operation in the process; (3) Uncertainty and sensitivity analysis, performed to identify the critical operational variables and parameters in the process. The uncertainty analysis is carried out using the Monte-Carlo technique. Sensitivity analysis employs the standardized regression coefficient (SRC) method, which provides a global sensitivity measure, βi, thereby showing how much each parameter contributes to the variance (uncertainty) of the model predictions. Thus, identifying the most critical parameters involved in the process, suitable for further analysis of the bioprocess. The uncertainty and sensitivity analysis identified the following most critical variables and parameters involved in the lignocellulosic ethanol production case study. For the operating cost, the enzyme loading showed the strongest impact, while reaction volume showed a significant impact on the ethanol/biomass ratio. The results showed also that it is possible to find a better alternative operation of the plant in comparison with the base case.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Meyer, A. S., Gernaey, K., Sin, G.
Publication date: 2011

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Bibliographical note
Modelling Framework for the Identification of Critical Variables and Parameters under Uncertainty in the Bioethanol Production from Lignocellulose

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State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Meyer, A. S., Gernaey, K., Sin, G.
Publication date: 2011
Peer-reviewed: Yes
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Bibliographical note

Model predictive control for plant-wide control of a reactor-separation-recycle system

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Contributors: Bialas, D. J., Huusom, J. K., Jørgensen, J. B., Sin, G.
Publication date: 2011
Peer-reviewed: No
Source: orbit
Research output: Research › Peer-review › Poster – Annual report year: 2011

Modified calibration protocol evaluated in a model-based testing of SBR flexibility
The purpose of this paper is to refine the BIOMATH calibration protocol for SBR systems, in particular to develop a pragmatic calibration protocol that takes advantage of SBR information-rich data, defines a simulation strategy to obtain proper initial conditions for model calibration and provides statistical evaluation of the calibration outcome. The updated calibration protocol is then evaluated on a case study to obtain a thoroughly validated model for testing the flexibility of an N-removing SBR to adapt the operating conditions to the changing influent wastewater load. The performance of reference operation using fixed phase length and dissolved oxygen set points and two real-time control strategies is compared to find optimal operation under dynamic conditions. The results show that a validated model of high quality is obtained using the updated protocol and that the optimization of the system’s performance can be achieved in different manners by implementing the proposed control strategies.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, University of Girona, Ghent University
Contributors: Corominas, L., Sin, G., Puig, S., Balaguer, M. D., Vanrolleghem, P. A., Colprim, J.
Pages: 205-214
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Bioprocess and Biosystems Engineering
Volume: 34
Multi-enzyme catalyzed processes: Next generation biocatalysis

Biocatalysis has been attracting increasing interest in recent years. Nevertheless, most studies concerning biocatalysis have been carried out using single enzymes (soluble or immobilized). Currently, multiple enzyme mixtures are attractive for the production of many compounds at an industrial level. In this review, a classification of multienzyme-catalyzed processes is proposed. Special emphasis is placed on the description of multienzyme ex-vivo systems where several reactions are carried out by a combination of enzymes acting outside the cell. Furthermore, reaction and process considerations for mathematical modeling are discussed for the specific case where the synthetic reactions are carried out in a single reactor, the so-called multienzyme ‘in-pot’ process. In addition, options for multienzyme ‘in-pot’ process improvements via process engineering and enzyme immobilization technology are described. Finally, enzyme modification via protein engineering is also discussed, such that a better compatibility of the enzymes in the reactor is achieved as a means of assisting the implementation of multienzyme ‘in-pot’ processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Andrade Santacoloma, P. D. G., Sin, G., Gernaey, K., Woodley, J.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.95 SJR 1.405 SNIP 0.978
Web of Science (2017): Impact factor 3.584
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.48 SJR 1.068 SNIP 0.85
Web of Science (2016): Impact factor 2.857
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.54 SJR 1.301 SNIP 1.01
Web of Science (2015): Impact factor 2.922
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.38 SJR 1.033 SNIP 0.982
Web of Science (2014): Impact factor 2.528
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.44 SJR 1.135 SNIP 0.967
Web of Science (2013): Impact factor 2.549
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.32 SJR 1.203 SNIP 1.128
Web of Science (2012): Impact factor 2.739
ISI indexed (2012): ISI indexed yes
Multivariate Principal Component Analysis and Case-Based Reasoning for monitoring, fault detection and diagnosis in a WWTP

The main idea of this paper is to develop a methodology for process monitoring, fault detection and predictive diagnosis of a WasteWater Treatment Plant (WWTP). To achieve this goal, a combination of Multiway Principal Component Analysis (MPCA) and Case-Based Reasoning (CBR) is proposed. First, MPCA is used to reduce the multi-dimensional nature of online process data, which summarises most of the variance of the process data in a few (new) variables. Next, the outputs of MPCA (t-scores, Q-statistic) are provided as inputs (descriptors) to the CBR method, which is employed to identify problems and propose appropriate solutions (hence diagnosis) based on previously stored cases. The methodology is evaluated on a pilot-scale SBR performing nitrogen, phosphorus and COD removal and to help to diagnose abnormal situations in the process operation. Finally, it is believed that the methodology is a promising tool for automatic diagnosis and real-time warning, which can be used for daily management of plant operation.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, University of Girona
Contributors: Ruiz, M., Sin, G., Berjaga, X., Colprim, J., Puig, S., Colomer, J.
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Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Web of Science (2012): Impact factor 1.102
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.25 SJR 0.594 SNIP 0.631
Web of Science (2011): Impact factor 1.122
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.529 SNIP 0.597
Web of Science (2010): Impact factor 1.056
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.592 SNIP 0.693
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.583 SNIP 0.694
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.736 SNIP 0.766
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.696 SNIP 0.789
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.767 SNIP 0.841
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.875 SNIP 0.897
Web of Science (2004): Indexed yes
Uncertainty derived from one of the process models – such as one-dimensional secondary settling tank (SST) models – can impact the output of the other process models, e.g., biokinetic (ASM1), as well as the integrated wastewater treatment plant (WWTP) models. The model structure and parameter uncertainty of settler models can therefore propagate, and add to the uncertainties in prediction of any plant performance criteria. Here we present an assessment of the relative significance of secondary settling model performance in WWTP simulations. We perform a global sensitivity analysis (GSA) based on Monte Carlo analysis in combination with multi-linear regression using four different simulation scenarios. We use the Benchmark Simulation Model Nr. 1 (BSM1), in which, we consider two operation scenarios for wastage of activated sludge (WAS), i.e. from the recycle of activated sludge (RAS) stream and from the last aerobic bioreactor upstream to the SST (Garrett/hydraulic method). For model structure uncertainty, two one-dimensional secondary settling tank (1-D SST) models are assessed, including a first-order model (the widely used Takács-model), in which the feasibility of using measured parameters for calibration is limited. The other SST model is a state-of-the-art, second-order, convection-dispersion tool (Plósz et al., 2007). The sensitivity results obtained from the four scenarios consistently indicate that the settler models and their parameters are among the most significant sources of uncertainty contributing to the predicted plant effluent data as well as sludge production and aeration demand, followed by influent wastewater fractions and biokinetic parameters, especially for autotrophs. Additionally, our results show that the first-order model systematically underrepresents uncertainty. The outcome of this study contributes to a better understanding of uncertainty in WWTPs, and explicitly demonstrates the significance of secondary settling processes that are crucial elements of model prediction under dry and wet-weather loading conditions.
Systematic Modelling and Crystal Size Distribution Control for Batch Crystallization Processes

Crystallization processes are an important class of separation methods that are frequently used in the chemical, the pharmaceutical and the food industry. The specifications of the crystal product are usually given in terms of crystal size, shape and purity. In order to predict the desired crystal morphology by means of model-based approaches, appropriate models covering the effects of the various operational parameters on the behavior of the crystals are necessary. Usually the main difficulty in batch crystallization is to accomplish a uniform CSD. There are many ways to enhance the control of CSD such as to use supersaturation control which drives the process within the metastable zone or by determining the amount and size of seeds that should be added into a crystallizer through seed recipe design approach. Therefore, there is a need for a generic crystallization model that can provide a better understanding of crystallization operations and from which a large number of specific models for different crystallization processes can be generated. Furthermore, to control and monitor the crystallization operations and to ensure that the desired CSD is achieved, an appropriate Process Analytical Technology (PAT) system needs to be available. That is, the design of process control and product monitoring system that will obtain the desired end-product properties is also needed. The generic multi-dimensional model-based framework of batch cooling crystallization processes has been developed covering a wide range of crystallization models and operational scenarios. The use of the generic model will be illustrated, in this paper, through the ICAS-PAT software for design of process monitoring and control system. ICAS-PAT consists of a model library and a knowledge base that allows the user to design/validate PAT systems through a systematic computer aided framework. The generic crystallizer model has been implemented in the ICAS-PAT model library. The application of the model-based framework will be highlighted through a batch cooling crystallization processes where the objective is to obtain a desired CSD. In order to predict the desired CSD at the end of the batch, an analytical CSD estimator based on the assumption of the constant supersaturation will be employed. Through this estimator, supersaturation set-point can be identified indicating that by maintaining the supersaturation at its set-point will result into achieving the specified CSD consistently. Thus using the ICAS-PAT, the crystallization operations can be monitored and controlled according to the required set-point during the batch run. For this purpose, the generation of the needed crystallization model will illustrated together with its use in the ICAS-PAT software. Crystallization processes form an important class of separation methods that are frequently used in the chemical, the pharmaceutical and the food industry. The specifications of the crystal product are usually given in terms of crystal size, shape and purity. In order to predict the desired crystal morphology by means of model-based approaches, appropriate models covering the effects of the various operational parameters on the behavior of the crystals are necessary. Usually the main difficulty in batch crystallization is to accomplish a uniform CSD. There are many ways to enhance the control of CSD such as to use supersaturation control which drives the process within the metastable zone or by determining the amount and size of seeds that should be added into a crystallizer through seed recipe design approach. Therefore, there is a need for a generic crystallization model that can provide a better understanding of crystallization operations and from which a large number of specific models for different crystallization processes can be generated. Furthermore, to control and monitor the crystallization operations and to ensure that the desired CSD is achieved, an appropriate Process Analytical Technology (PAT) system needs to be available. That is, the design of process control and product monitoring system that will obtain the desired end-product properties is also needed.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, University of Illinois at Chicago
Contributors: Abdul Samad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
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Systematic multi-scale model development strategy for fragrance spraying process and transport

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Firmenich Inc.
Contributors: Heitzig, M., Gregson, C., Sin, G., Gani, R.
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Peer-reviewed: Yes
Event: Abstract from 8th European Congress of Chemical Engineering, Berlin, Germany.
Electronic versions:
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Systematic procedure for generating operational policies to achieve target crystal size distribution (CSD) in batch cooling crystallization

A systematic procedure to achieve a target crystal size distribution (CSD) under generated operational policies in batch cooling crystallization is presented. An analytical CSD estimator has been employed in the systematic procedure to generate the necessary operational policies to achieve the target CSD. Furthermore, this systematic procedure has been integrated with a generic multi-dimensional model-based framework. The generic nature of the model-based framework allows the study of a wide range of chemical systems under different operational scenarios, enabling thereby, the analysis of various crystallization operations and conditions. Therefore this generic multidimensional model-based framework can be used to generate "specific" models for crystallization processes and further verify the operational policies generated by the analytical CSD estimator for achieving the targeted CSD consistently. The application of the systematic procedure is illustrated for a potassium dichromate case study.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abdul Samad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
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Research output: Research - peer-review › Article in proceedings – Annual report year: 2011

Systematic Procedure for Generating Operational Policies to Achieve Target Crystal Size Distribution (CSD) in Batch Cooling Crystallization

Batch cooling crystallization is one of the important unit operations involving separation of solid-liquid phases. Usually the most common crystal product qualities are directly related to the crystal size distribution (CSD). However the main difficulty in batch crystallization is to obtain a uniform and reproducible CSD. Therefore supersaturation control can be applied to drive the process within the metastable zone and thereby enhance the control of the CSD. Although this approach has been shown to produce high quality crystals, the set point operating profiles for the supersaturation controller are usually chosen arbitrarily or by trial-and-error. Therefore there is a need for a systematic procedure to generate operational policy that guarantees the target CSD can be achieved. Furthermore, to predict the desired crystal morphology by means of model-based approaches, appropriate models covering the effects of the various operational parameters on the behavior of the crystals are necessary. That is, generic multi-dimensional model-based framework that covers a wide range of crystallization models and operational scenarios. The objectives of this work are to develop a systematic procedure for generating operational policies to achieve target CSD for batch cooling crystallization. In this procedure, an analytical CSD estimator will be employed to generate an operational policy. The estimator is based on the assumptions of constant supersaturation and an operation that is dominated by size dependent growth. The generated operational policy provides the supersaturation set point and by maintaining the operation at this point, a target CSD is
achieved. Different operational policies that yield the same target CSD are then generated and compared with the CSD performance. All the operational policies generated by analytical CSD estimators are in this way validated with closed loop control. Here the generic multi-dimensional model-based framework for batch cooling crystallization has been developed and integrated with the monitoring and control procedure. Through this generic multi-dimensional model-based framework, a "specific" model can be generated and be used for closed loop control to verify the operation policies. Finally the performance between simulation models and analytical estimators will be compared and the best performance will be analyzed in term of CSD obtained, mean size diameter and total crystal mass. In this paper, the application of systematic procedure is illustrated for the potassium dichromate case study.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abdul Samad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
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Technology Evaluation of Process Configurations for Second Generation Bioethanol Production using Dynamic Model-based Simulations
An assessment of a number of different process flowsheets for bioethanol production was performed using dynamic model-based simulations. The evaluation employed diverse operational scenarios such as, fed-batch, continuous and continuous with recycle configurations. Each configuration was evaluated against the following benchmark criteria, yield (kg ethanol/kg dry-biomass), final product concentration and number of unit operations required in the different process configurations. The results has shown the process configuration for simultaneous saccharification and co-fermentation (SSCF) operating in continuous mode with a recycle of the SSCF reactor effluent, results in the best productivity of bioethanol among the proposed process configurations, with a yield of 0.18 kg ethanol /kg dry-biomass.

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State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Meyer, A. S., Gernaey, K., Sin, G.
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Technology Evaluation of Process Configurations for Second Generation Bioethanol Production using Dynamic Model-based Simulations

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State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Meyer, A. S., Gernaey, K., Sin, G.
Publication date: 2011
Peer-reviewed: Yes
Towards benchmarking of multivariable controllers in chemical/biochemical industries: Plantwide control for ethylene glycol production

In this paper we discuss a simple yet realistic benchmark plant for evaluation and comparison of advanced multivariable control for chemical and biochemical processes. The benchmark plant is based on recycle-separator-recycle systems for ethylene glycol production and implemented in Matlab-Simulink platform. The benchmark plant is used to illustrate a procedure for plantwide control design in which Model Predictive Control (MPC) is evaluated and compared to a control structure based on single-input/single-output PID-controllers. We believe such a benchmark plant has a promising potential for education purposes (operator training, student education, etc) as well as scientific research into chemical process control where it enables rapid evaluation and comparison of advanced multivariable controllers as demonstrated in this study.

Uncertainty and Sensitivity Analysis of Filtration Models for Non-Fickian transport and Hyperexponential deposition

Uncertainty and sensitivity analyses are carried out to investigate the predictive accuracy of the filtration models for describing non-Fickian transport and hyperexponential deposition. Five different modeling approaches, involving the elliptic equation with different types of distributed filtration coefficients and the CTRW equation expressed in Laplace space, are selected to simulate eight experiments. These experiments involve both porous media and colloid-medium interactions of different heterogeneity degrees. The uncertainty of elliptic equation predictions with distributed filtration coefficients is larger than that with a single filtration coefficient. The uncertainties of model predictions from the elliptic equation and CTRW equation in Laplace space are minimal for solute transport. Higher uncertainties of parameter estimation and model outputs are observed in the cases with the porous media and the colloid-medium interactions of higher heterogeneity. The parameters for the distribution of filtration coefficients could not be uniquely identified due to strong correlations. In the cases of heterogeneous colloid-medium interactions where hyper-exponential deposition is observed, the distribution of filtration coefficients could not be accurately determined by the effluent concentration profile alone. Measurements of deposition are necessary. The effluent concentrations around the breakthrough and around the end of colloid injection are more sensitive to dispersion coefficients than filtration coefficients, while deposition is more sensitive to filtration coefficients. More experimental measurements at these moments are suggested to determine dispersion coefficients more accurately. More measurements of the steady-state effluent concentration or deposition are suggested to determine filtration coefficients more accurately.
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Volume: 168
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.01
Web of Science (2017): Impact factor 6.735
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.34
Web of Science (2016): Impact factor 6.216
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.68
Web of Science (2015): Impact factor 5.31
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
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.92
Web of Science (2012): Impact factor 3.473
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.96
Web of Science (2011): Impact factor 3.461
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Impact factor 3.074
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
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Validation of Inhibition Effect in the Cellulose Hydrolysis: a Dynamic Modelling Approach

Enzymatic hydrolysis is one of the main steps in the processing of bioethanol from lignocellulosic raw materials. However, complete understanding of the underlying phenomena is still under development. Hence, this study has focused on validation of the inhibition effects in the cellulosic biomass hydrolysis employing a dynamic mathematical model. A systematic framework for parameter estimation is used for model validation, which helps overcome the problem of parameter correlation. Data sets obtained from carefully designed enzymatic cellulose and cellobiose hydrolysis experiments, were used for parameter estimation (calibration) and validation purposes. The model predictions using calibrated parameters have shown good agreement with the validation data sets, which provides credibility to the model structure and the parameter values.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
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Validation of Inhibition Effect in the Cellulose Hydrolysis: a Dynamic Modelling Approach

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Tsai, C., Meyer, A. S., Gernaey, K., Sin, G.
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Peer-reviewed: Yes
Event: Poster session presented at AMIDIQ 32nd National Meeting and 1st International Congress, Riviera Maya, Mexico.
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Wastewater Systems

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Ghent University, Lund University
Contributors: Gernaey, K., Nopens, I., Sin, G., Jeppsson, U.
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Publication date: 2011
**Wastewater treatment models**

The state-of-the-art level reached in modeling wastewater treatment plants (WWTPs) is reported. For suspended growth systems, WWTP models have evolved from simple description of biological removal of organic carbon and nitrogen in aeration tanks (ASM1 in 1987) to more advanced levels including description of biological phosphorus removal, physical-chemical processes, hydraulics and settling tanks. For attached growth systems, biofilm models have progressed from analytical steady-state models to more complex 2D/3D dynamic numerical models. Plant-wide modeling is set to advance further the practice of WWTP modeling by linking the wastewater treatment line with the sludge handling line in one modeling platform. Application of WWTP models is currently rather time consuming and thus expensive due to the high model complexity, and requires a great deal of process knowledge and modeling expertise. Efficient and good modeling practice therefore requires the use of a proper set of guidelines, thus grounding the modeling studies on a general and systematic framework. Last but not least, general limitations of WWTP models – more specifically activated sludge models – are introduced since these define a boundary of validity for WWTP model applications.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Gernaey, K., Sin, G.
Number of pages: 5,320
Publication date: 2011

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Sin, G., Glarborg, P., Gani, R.
Publication date: 2010

Event information
Event: 6th International Conference on Sensitivity Analysis of Model Output
Location: Milan, Italy, 19-22 July
Source: orbit
Source-ID: 265931
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

A computer-aided modelling framework for use in product-process engineering

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Sin, G., Glarborg, P., Gani, R.
Publication date: 2010

Event information
Event: 19th International Congress of Chemical and Process Engineering and 7th European Congress of Chemical Engineering
Location: Prague, Czech Republic
Source: orbit
Source-ID: 267044
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

A Dynamic Model for Cellulosic Biomass Hydrolysis: Validation of Hydrolysis and Product Inhibition Mechanism

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for BioProcess Engineering
Contributors: Eeclo, J., Tsai, C., Morales Rodriguez, R., Gernaey, K., Meyer, A. S., Sin, G.
Publication date: 2010

Event information
Event: 2010 AIChE Annual Meeting
Location: Salt Lake City, United States
Source: orbit
Source-ID: 268894
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010
A Generic Model-Based Framework for Batch Cooling Crystallization Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abdul Samad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
Publication date: 2010
Peer-reviewed: Yes
Source: orbit
Source-ID: 267052
Research output: Research - peer-review › Poster – Annual report year: 2010

A Generic Multi-Dimensional Model-Based Framework for Batch Cooling Crystallization Process

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abdul Samad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
Publication date: 2010

Event information
Event: 2010 AIChE Annual Meeting
Location: Salt Lake City, United States
Source: orbit
Source-ID: 268879
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

A Model-Based Methodology for Simultaneous Design and Control of a Bioethanol Production Process
In this work, a framework for the simultaneous solution of design and control problems is presented. Within this framework, two methodologies are presented, the integrated process design and controller design (IPDC) methodology and the process-group contribution (PGC) methodology. The concepts of attainable region (AR), driving force (DF), process-group (PG) and reverse simulation are used within these methodologies. The IPDC methodology is used to find the optimal design-control strategy of a process by locating the maximum point in the AR and DF diagrams for reactor and separator, respectively. The PGC methodology is used to generate more efficient separation designs in terms of energy consumption by targeting the separation task at the largest DF. Both methodologies are highlighted through the application of two case studies, a bioethanol production process and a succinic acid production process. In the final discussion, the results are put in context.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for BioProcess Engineering
Pages: 2043-2061
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Peer-reviewed: Yes

Publication information
Journal: Computers & Chemical Engineering
Volume: 34
Issue number: 12
ISSN (Print): 0098-1354
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
Web of Science (2017): Impact factor 3.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
A New Extant Respirometric Assay to Estimate Intrinsic Growth Parameters Applied to Study Plasmid Metabolic Burden

Start-Lip phenomena in microbial biokinetic assays are not captured by the most commonly used growth-related equations. In this Study we propose a new respirometric experimental design to estimate intrinsic growth parameters that allow us to avoid these limitations without data omission, separate mathematical treatment, or wake-up pulses prior to the analysis. Identifiability and sensitivity analysis were performed to confirm the robustness of the new approach for obtaining unique and accurate estimates of growth kinetic parameters. The new experimental design was applied to establish the metabolic burden caused by the carriage of a pWW0 TOL plasmid in the model organism Pseudomonas putida KT2440. The metabolic burden associated was manifested as a reduction in the yield and the specific growth rate of the host, with both plasmid maintenance and the over-expression of recombinant proteins from the plasmid contributing equally to the overall effect. Biotechnol. Bioeng. 2010;105: 141-149. (C) 2009 Wiley Periodicals, Inc.

General information
State: Published
Organisations: Department of Environmental Engineering, Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Environmental Chemistry
Contributors: Seoane, J. M., Sin, G., Lardon, L., Gernaey, K., Smets, B. F.
Pages: 141-149
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Biotechnology and Bioengineering (Print)
Volume: 105
Issue number: 1
ISSN (Print): 0006-3592
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.07 SJR 1.372 SNIP 1.186
Web of Science (2017): Impact factor 3.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.447 SNIP 1.178
Web of Science (2016): Impact factor 4.481
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.44 SJR 1.632 SNIP 1.355
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.16 SJR 1.612 SNIP 1.395
Web of Science (2014): Impact factor 4.126
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.44 SJR 1.637 SNIP 1.427
Web of Science (2013): Impact factor 4.164
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.04 SJR 1.62 SNIP 1.364
Web of Science (2012): Impact factor 3.648
ISI indexed (2012): ISI indexed yes
Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problem for Reactor-Separator-Recycle System

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abd. Hamid, M., Sin, G., Gani, R.
Pages: 148-149
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemieningeniørkonference 2010
Source: orbit
Source-ID: 266240
Research output: Research › Article in proceedings – Annual report year: 2010
Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problem for Reactor-Separator-Recycle System

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abd.Hamid, M., Sin, G., Gani, R.
Publication date: 2010
Source: orbit
Source-ID: 266267
Research output: Research › Poster – Annual report year: 2010

This paper presents the integrated process design and controller design (IPDC) for a reactor-separator-recycle (RSR) system and evaluates a decomposition methodology to solve the IPDC problem. Accordingly, the IPDC problem is solved by decomposing it into four hierarchical stages: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, and (iv) final selection and verification. The methodology makes use of thermodynamic-process insights and the reverse design approach to arrive at the final process-controller design decisions. The developed methodology is illustrated through the design of a RSR system involving consecutive reactions, A → B → C and shown to provide effective solutions that satisfy design, control and cost criteria. The advantage of the proposed methodology is that it is systematic, makes use of thermodynamic-process knowledge and provides valuable insights to the solution of IPDC problems for RSR systems.

Host publication information
Source: orbit
Source-ID: 265043
Research output: Research › peer-review › Article in proceedings – Annual report year: 2010

Event information
Event: CAPE Forum 2010
Location: Aachen, Germany
Source: orbit
Source-ID: 265119
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010


General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abd.Hamid, M., Sin, G., Gani, R.
Publication date: 2010

Event information
Event: CAPE Forum 2010
Location: Aachen, Germany
Source: orbit
Source-ID: 265119
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010
Application of mechanistic models to fermentation and biocatalysis for next-generation processes

Mechanistic models are based on deterministic principles, and recently, interest in them has grown substantially. Herein we present an overview of mechanistic models and their applications in biotechnology, including future perspectives. Model utility is highlighted with respect to selection of variables required for measurement, control and process design. In the near future, mechanistic models with a higher degree of detail will play key roles in the development of efficient next-generation fermentation and biocatalytic processes. Moreover, mechanistic models will be used increasingly in the frame of multi-objective decision-making under uncertainty and to promote increased selectivity of products.
Assessing Reliability of Cellulose Hydrolysis Models to Support Biofuel Process Design – Identifiability and Uncertainty Analysis

The reliability of cellulose hydrolysis models is studied using the NREL model. An identifiability analysis revealed that only 6 out of 26 parameters are identifiable from the available data (typical hydrolysis experiments). Attempting to identify a higher number of parameters (as done in the original NREL model publication) results in significant errors on the parameter estimates. The reasons for this poor identifiability are related to (i) model structure complexity, inherently containing correlated parameters due to Michaelis–Menten type kinetics, and (ii) the available data, which are not informative enough (sensitivities of 16 parameters were insignificant). This indicates that the NREL model has severe parameter uncertainty, likely to be the case for other hydrolysis models as well since similar kinetic expressions are used. To overcome this impasse, we have used the Monte Carlo procedure to analyze the uncertainty of model predictions. This allows judging the fitness of the model to the purpose under uncertainty. Hence we recommend uncertainty analysis as a proactive solution when faced with model uncertainty, which is the case for biofuel process development research.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Sin, G., Meyer, A. S., Gernaey, K.
Pages: 1385-1392
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Computers & Chemical Engineering
Volume: 34
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ISSN (Print): 0098-1354
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
Web of Science (2017): Impact factor 3.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1 SNIP 1.631
Web of Science (2016): Impact factor 3.024
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.713
Web of Science (2015): Impact factor 2.581
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.22 SJR 1.168 SNIP 1.728
Web of Science (2014): Impact factor 2.784
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.06 SJR 1.21 SNIP 1.744
Web of Science (2013): Impact factor 2.452
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.05 SJR 1.138 SNIP 1.897
Web of Science (2012): Impact factor 2.091
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.8 SJR 1.144 SNIP 1.736
Web of Science (2011): Impact factor 2.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.167 SNIP 1.752
Web of Science (2010): Impact factor 2.072
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.171 SNIP 2.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.288 SNIP 2.094
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.621 SNIP 1.916
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.306 SNIP 1.888
Scopus rating (2005): SJR 1.306 SNIP 1.882
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.112 SNIP 1.86
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.332 SNIP 1.884
Scopus rating (2002): SJR 0.8 SNIP 0.916
A systematic approach for fine-tuning of fuzzy controllers applied to WWTPs

A systematic approach for fine-tuning fuzzy controllers has been developed and evaluated for an aeration control system implemented in a WWTR. The challenge with the application of fuzzy controllers to WWTPs is simply that they contain many parameters, which need to be adjusted for different WWTP applications. To this end, a methodology based on model simulations is used that employs three statistical methods: (i) Monte-Carlo procedure: to find proper initial conditions, (ii) Identifiability analysis: to find an identifiable parameter subset of the fuzzy controller and (iii) minimization algorithm: to fine-tune the identifiable parameter subset of the controller. Indeed, the initial location found by Monte-Carlo simulations provided better results than using trial and error approach when identifying parameters of the fuzzy controller. The identifiable subset was reduced to 4 parameters from a total of 33, which improved the quality of the optimization of the control system by a minimization algorithm. Overall the systematic approach considerably improved the performance of the control system as measured by the Integral Absolute Error (deviation between the set-point and the controlled variable) of the controllers. Moreover, the methodology overcomes the dependency of the initial parameter space issue typical of local identifiability analysis. All in all this systematic approach is expected to facilitate the design and application of fuzzy controllers in particular to WWTPs compared to the time-consuming and tedious trial and error approach currently used in practice. © 2009 Elsevier Ltd. All rights reserved.
Computer-Aided Modelling for Efficient and Innovative Product-Process Engineering

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Sin, G., Glarborg, P., Gani, R.
Pages: 171-172
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Source: orbit
Control of Process Operations and Monitoring of Product Qualities through Generic Model-based in Batch Cooling Crystallization

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Abdul Samad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
Publication date: 2010

Event information
Event: 20th European Symposium on Computer Aided Process Engineering
Location: Ischia, Italy
Source: orbit
Source-ID: 265226
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Control of Process Operations and Monitoring of Product Qualities through Generic Model-based in Batch Cooling Crystallization

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Abdul Samad, N. A. F., Singh, R., Sin, G., Gernaey, K., Gani, R.
Pages: 613-618
Publication date: 2010

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 28
Publisher: Elsevier
ISBN (Print): 04-44-53569-1
URLs: http://www.elsevierdirect.com/product.jsp?isbn=9780444535696&dmnum=CWS1
Source: orbit
Source-ID: 255451
Research output: Research › peer-review › Article in proceedings – Annual report year: 2010

Development of a mathematical model describing hydrolysis and co-fermentation of C6 and C5 sugars

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Gernaey, K., Meyer, A. S., Sin, G.
Publication date: 2010

Event information
Event: 2nd International Symposium on Sustainable Chemical Product and Process Engineering
Location: Hangzhou, China
Source: orbit
Source-ID: 265204
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Development of a mathematical model describing hydrolysis and co-fermentation of C6 and C5 sugars
Reliable production of biofuels and specifically bioethanol has attracted a significant amount of research recently. Within this context, this study deals with dynamic simulation of bioethanol production processes and in particular aims at developing a mathematical model for describing simultaneous saccharification and co-fermentation (SSCF) of C6 and C5 sugars. Model construction has been carried out by combining existing mathematical models for enzymatic hydrolysis on
the one hand and co-fermentation on the other hand. An inhibition of ethanol on cellulose conversion was introduced in order to increase the degree of reliability. The mathematical model for the SSCF has been tested for a modified version of the process flowsheet proposed by the National Renewable Energy Laboratory (NREL). The model can now be used to evaluate different process configurations for 2G bioethanol production using corn stover as a feedstock.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Gernaey, K., Meyer, A. S., Sin, G.
Publication date: 2010

**Host publication information**
Title of host publication: 2. International Symposium on Sustainable Chemical Product and Process Engineering
Keywords: Plant-wide, SSCF, Corn stover, Second generation, Dynamic modeling, Bioethanol
Electronic versions:
PEC10-67.pdf

**Bibliographical note**
Electronic version: 48. E-01
Source: orbit
Source-ID: 276751
Research output: Research - peer-review › Article in proceedings – Annual report year: 2011

**Dynamic plant-wide modelling for bioethanol production from lignocellulosic biomass (2G)**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Gernaey, K., Meyer, A. S., Sin, G.
Publication date: 2010

**Event information**
Event: 19th International Congress of Chemical and Process Engineering and 7th European Congress of Chemical Engineering
Location: Prague, Czech Republic
Source: orbit
Source-ID: 267043
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

**Feasibility of the batch fermentation process of Ricotta Cheese Whey (RCW)**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Sansonetti, S., Curcio, S., Calabrò, V., Sin, G., Iorio, G.
Pages: 79-84
Publication date: 2010

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Volume: 20
Source: orbit
Source-ID: 264995
Research output: Research - peer-review › Article in proceedings – Annual report year: 2010

**From lab experiments to plant operation and design: Bioethanol production from lignocellulose using different enzyme technologies**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
ICAS-MoT, a Computer-Aided Modeling Tool

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Sin, G., Glarborg, P., Gani, R.
Publication date: 2010

Event information
Event: 2010 AIChE Annual Meeting
Location: Salt Lake City, United States
Source: orbit
Source-ID: 268893
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Integrated Dynamic Plant-Wide Model-Based Simulation of Bioethanol Production from Lignocellulose

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Gernaey, K., Meyer, A. S., Sin, G.
Pages: 192-193
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Source: orbit
Source-ID: 266245
Research output: Research › Article in proceedings – Annual report year: 2010

Integrated Dynamic Plant-Wide Model-Based Simulation of Bioethanol Production from Lignocellulose

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Gernaey, K., Meyer, A. S., Sin, G.
Publication date: 2010
Peer-reviewed: No
Source: orbit
Source-ID: 266272
Research output: Research › Poster – Annual report year: 2010

Integrated Dynamic Plant-Wide Model-Based Simulation of Bioethanol Production from Lignocellulose

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Gernaey, K., Meyer, A. S., Sin, G.
Integration of process design and controller design for chemical processes using model-based methodology

In this paper, a novel systematic model-based methodology for performing integrated process design and controller design (IPDC) for chemical processes is presented. The methodology uses a decomposition method to solve the IPDC typically formulated as a mathematical programming (optimization with constraints) problem. Accordingly the optimization problem is decomposed into four sub-problems: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, and (iv) final selection and verification, which are relatively easier to solve. The methodology makes use of thermodynamic-process insights and the reverse design approach to arrive at the final process design–controller design decisions. The developed methodology is illustrated through the design of: (a) a single reactor, (b) a single separator, and (c) a reactor–separator-recycle system and shown to provide effective solutions that satisfy design, control and cost criteria. The advantage of the proposed methodology is that it is systematic, makes use of thermodynamic-process knowledge and provides valuable insights to the solution of IPDC problems in chemical engineering practice.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Abd.Hamid, M., Sin, G., Gani, R.
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Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Computers & Chemical Engineering
Volume: 34
Issue number: 5
ISSN (Print): 0098-1354
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.65 SJR 1.024 SNIP 1.613
Web of Science (2017): Impact factor 3.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1 SNIP 1.631
Web of Science (2016): Impact factor 3.024
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.04 SJR 1.108 SNIP 1.713
Web of Science (2015): Impact factor 2.581
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.22 SJR 1.168 SNIP 1.728
Web of Science (2014): Impact factor 2.784
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.06 SJR 1.21 SNIP 1.744
Web of Science (2013): Impact factor 2.452
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.05 SJR 1.138 SNIP 1.897
Web of Science (2012): Impact factor 2.091
IWA Design and Operational Uncertainty Task Group: Document and evaluate existing methods for assessing and evaluating uncertainty in wastewater treatment

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Sprouse, G., McCormick, J., Schraa, O., Sin, G.
Publication date: 2010

Event information
Event: IWA World Water Congress & Exhibition
Location: Montréal, Canada
Source: orbit
Source-ID: 266495
Research output: Research - peer-review › Journal article – Annual report year: 2010
Managing Multi-Scale Modeling Issues in Chemical Engineering - a Computer-Aided Framework

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Sin, G., Glarborg, P., Gani, R.
Publication date: 2010

Event information
Event: 2010 AIChE Annual Meeting
Location: Salt Lake City, United States
Source: orbit
Source-ID: 268878
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Model predictive control for plant-wide control of a reactor-separator-recycle system

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Contributors: Bialas, D. J., Huusom, J. K., Jørgensen, J. B., Sin, G.
Publication date: 2010

Event information
Event: 16th Nordic Process Control Workshop
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Source: orbit
Source-ID: 266529
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Model predictive control for reactor-separator-recycle system

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Contributors: Bialas, D. J., Huusom, J. K., Jørgensen, J. B., Sin, G.
Number of pages: 145
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiiingeniørkonference 2010
Source: orbit
Source-ID: 265907
Research output: Research › Article in proceedings – Annual report year: 2010

Model predictive control for reactor-separator-recycle system

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Contributors: Bialas, D. J., Huusom, J. K., Jørgensen, J. B., Sin, G.
Publication date: 2010
Peer-reviewed: No
Source: orbit
Source-ID: 265908
Research output: Research › Poster – Annual report year: 2010
New concepts for multi-enzymatic synthetic processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Andrade Santacoloma, P. D. G., Sin, G., Gernaey, K., Woodley, J.
Pages: 182-183
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Source: orbit
Source-ID: 266249
Research output: Research › Article in proceedings – Annual report year: 2010

New concepts for multi-enzymatic synthetic processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Andrade Santacoloma, P. D. G., Sin, G., Gernaey, K., Woodley, J.
Publication date: 2010

Event information
Event: BEST 2010
Location: Bologna, Italy
Source: orbit
Source-ID: 267264
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

New concepts for multi-enzymatic synthetic processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Andrade Santacoloma, P. D. G., Sin, G., Gernaey, K., Woodley, J.
Publication date: 2010
Peer-reviewed: No
Source: orbit
Source-ID: 266276
Research output: Research › Poster – Annual report year: 2010

Perspectives on the use of global uncertainty and sensitivity analysis methods in a PAT context

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Microbial Biotechnology, Department of Systems Biology
Contributors: Sin, G., Eliasson Lantz, A., Gernaey, K.
Publication date: 2010

Event information
Event: 24th International Foundation Process Analytical Chemistry (IFPAC®)
Location: Baltimore, Maryland, United States
Source: orbit
Source-ID: 265114
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Process Technology Evaluation for Lignocellulosic Bioethanol Production: Plantwide Configurations Using a Dynamic Modeling Approach

General information
Sensitivity analysis in the WWTP modelling community – new opportunities and applications

A mainstream viewpoint on sensitivity analysis in the wastewater modelling community is that it is a first-order differential analysis of outputs with respect to the parameters – typically obtained by perturbing one parameter at a time with a small factor. An alternative viewpoint on sensitivity analysis is related to uncertainty analysis, which attempts to relate the total uncertainty in the outputs to the uncertainty in the inputs. In this paper we evaluate and discuss two such sensitivity analysis methods for two different purposes/case studies: (i) Applying sensitivity analysis to a plant design (BSM1 plant layout) using Standardized Regression Coefficients (SRC) and (ii) Applying sensitivity analysis to help fine-tuning a fuzzy controller for a BNPR plant using Morris Screening. The results obtained from each case study are then critically discussed in view of practical applications of sensitivity analysis in day-to-day engineering projects.

Sensitivity Analysis of a Kinetic Model Describing the Bi-enzymatic Synthesis of Lactobionic Acid

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Andrade Santacoloma, P. D. G., Sin, G., Gernaey, K., Woodley, J.
Pages: 1491-1496
Publication date: 2010

Host publication information
Systematic model development for partial nitrification of landfill leachate in a SBR
This study deals with partial nitrification in a sequencing batch reactor (PN-SBR) treating raw urban landfill leachate. In order to enhance process insight (e.g., quantify interactions between aeration, CO2 stripping, alkalinity, pH, nitrification kinetics), a mathematical model has been set up. Following a systematic procedure, the model was successfully constructed, calibrated and validated using data from short-term (one cycle) operation of the PN-SBR. The evaluation of the model revealed a good fit to the main physical-chemical measurements (ammonium, nitrite, nitrate and inorganic carbon), confirmed by statistical tests. Good model fits were also obtained for pH, despite a slight bias in pH prediction, probably caused by the high salinity of the leachate. Future work will be addressed to the model-based evaluation of the interaction of different factors (aeration, stripping, pH, inhibitions, among others) and their impact on the process performance.
Uncertainty in modelling, design and operation of chemical processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Sin, G.
Publication date: 2010

Event information
Event: 3. Dansk KemiingeniørKonference
Location: Technical University of Denmark, Kgs. Lyngby, Denmark
Source: orbit
Source-ID: 266281
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Uncertainty in modelling, design and operation of chemical processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Sin, G.
Number of pages: 44
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Source: orbit
Source-ID: 266255
Research output: Research › Article in proceedings – Annual report year: 2010
A Computer-Aided Modelling Tool for Efficient Model Identification and Analysis

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Sin, G., Glarborg, P., Gani, R.
Publication date: 2009

Event information
Event: 2009 AIChE Annual Meeting
Location: Nashville, TN, United States
Source: orbit
Source-ID: 252818
Research output: Research › Sound/Visual production (digital) – Annual report year: 2009


General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Heitzig, M., Morales Rodriguez, R., Sin, G., Glarborg, P., Gani, R.
Publication date: 2009

Event information
Event: 2009 AIChE Annual Meeting
Location: Nashville, TN, United States
Source: orbit
Source-ID: 252826
Research output: Research › Sound/Visual production (digital) – Annual report year: 2009

A Model-Based Methodology for Simultaneous Design and Control of a Bioethanol Production Process

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for BioProcess Engineering
Publication date: 2009

Event information
Event: 10th International Symposium on Process System Engineering
Location: Salvador de Bahia, Brazil
Source: orbit
Source-ID: 248304
Research output: Research › Sound/Visual production (digital) – Annual report year: 2009

A Model-Based Methodology for Simultaneous Design and Control of a Bioethanol Production Process
A new model-based methodology for simultaneous design and control of reaction-separation systems with recycle

A New Model-Based Methodology for Simultaneous Design and Control of Reaction-Separation System with Recycle

Application of ICAS-PAT On Design of Process Monitoring and Control System for a Batch Cooling Crystallization Process through Hybrid Multiscale Model-Based Analysis
Application of modeling and simulation tools for the evaluation of biocatalytic processes: a future perspective

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Sin, G., Gernaey, K., Woodley, J.
Pages: 1529-1538
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Biotechnology Progress
Volume: 25
Issue number: 6
ISSN (Print): 8756-7938
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.12 SJR 0.676 SNIP 0.785
Web of Science (2017): Impact factor 1.947
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.12 SJR 0.699 SNIP 0.768
Web of Science (2016): Impact factor 1.986
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.07 SJR 0.729 SNIP 0.805
Web of Science (2015): Impact factor 2.167
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.2 SJR 0.812 SNIP 0.929
Web of Science (2014): Impact factor 2.149
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.16 SJR 0.768 SNIP 0.857
Web of Science (2013): Impact factor 1.883
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.35 SJR 0.831 SNIP 0.871
Web of Science (2012): Impact factor 1.853
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.4 SJR 0.917 SNIP 0.948
Web of Science (2011): Impact factor 2.34
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.997 SNIP 0.934
Web of Science (2010): Impact factor 2.178
A priori regression analysis for the calibration of complex dynamic models: application to an integrated biological, chemical and physical model of antibiotic production with S. coelicolor

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Sin, G., Gernaey, K.
Publication date: 2009

Host publication information
Title of host publication: Computer Aided Chemical Engineering, on CD
Source: orbit
Source-ID: 245072
Research output: Research - peer-review → Article in proceedings → Annual report year: 2009


General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Sin, G., Meyer, A. S., Gernaey, K.
Publication date: 2009

Event information
Location: Breckenridge, CO, United States
Source: orbit
Source-ID: 248177

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Sin, G., Meyer, A. S., Gernaey, K.
Pages: 93-106
Publication date: 2009

Comparison of the Modeling Approach between Membrane Bioreactor and Conventional Activated Sludge Processes
Activated sludge models (ASM) have been developed and largely applied in conventional activated sludge (CAS) systems. The applicability of ASM to model membrane bioreactors (MBR) and the differences in modeling approaches have not been studied in detail. A laboratory-scale MBR was modeled using ASM2d. It was found that the ASM2d model structure can still be used for MBR modeling. There are significant differences related to ASM modeling. First, a lower maximum specific growth rate for MBR nitrifiers was estimated. Independent experiments demonstrated that this might be attributed to the inhibition effect of soluble microbial products (SMP) at elevated concentration. Second, a greater biomass affinity to oxygen and ammonium was found, which was probably related to smaller MBR sludge flocs. Finally, the membrane throughput during membrane backwashing/relaxation can be normalized and the membrane can be modeled as a continuous flow-through point separator. This simplicity has only a minor effect on ASM simulation results; however, it significantly improved simulation speed. Water Environ. Res., 81, 432 (2009).

General information
State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Physics, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Department of Environmental Engineering
Contributors: Jiang, T., Sin, G., Spanjers, H., Nopens, I., Kennedy, M. D., van der Meer, W., Futselaar, H., Amy, G., Vanrolleghem, P.
Pages: 432-440
Publication date: 2009
Peer-reviewed: Yes

Publication Information
Journal: Water Environment Research
Volume: 81
Issue number: 4
ISSN (Print): 1061-4303
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.84 SJR 0.283 SNIP 0.312
Web of Science (2017): Impact factor 0.825
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.89 SJR 0.324 SNIP 0.443
Web of Science (2016): Impact factor 0.91
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.8 SJR 0.344 SNIP 0.493
Web of Science (2015): Impact factor 0.659
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.75 SJR 0.4 SNIP 0.537
Web of Science (2014): Impact factor 0.865
Determination of optimal design and control decisions for reactor-separator systems with recycle

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Abd.Hamid, M., Sin, G., Gani, R.
Pages: 593-602
Publication date: 2009

Host publication information
Title of host publication: Proceedings for FOCAPD-2009
Source: orbit
Source-ID: 231830
Research output: Research - peer-review › Article in proceedings – Annual report year: 2009
Determination of optimal design and control decisions for reactor-separator systems with recycle

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Abd.Hamid, M., Sin, G., Gani, R.
Publication date: 2009
Peer-reviewed: Yes
Source: orbit
Source-ID: 248176
Research output: Research - peer-review › Poster – Annual report year: 2009

Development of An Integrated Dynamic Model for Bioethanol Production From Lignocellulosic Biomass

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Contributors: Morales Rodriguez, R., Sin, G., Gernaey, K., Meyer, A. S.
Publication date: 2009

Event information
Event: 2009 AIChE Annual Meeting
Location: Nashville, TN, United States
Source: orbit
Source-ID: 252819
Research output: Research › Sound/Visual production (digital) – Annual report year: 2009

Good Modeling Practice for PAT Applications: Propagation of Input Uncertainty and Sensitivity Analysis
The uncertainty and sensitivity analysis are evaluated for their usefulness as part of the model-building within Process Analytical Technology applications. A mechanistic model describing a batch cultivation of Streptomyces coelicolor for antibiotic production was used as case study. The input uncertainty resulting from assumptions of the model was propagated using the Monte Carlo procedure to estimate the output uncertainty. The results showed that significant uncertainty exists in the model outputs. Moreover the uncertainty in the biomass, glucose, ammonium and base-consumption were found low compared to the large uncertainty observed in the antibiotic and off-gas CO2 predictions. The output uncertainty was observed to be lower during the exponential growth phase, while higher in the stationary and death phases - meaning the model describes some periods better than others. To understand which input parameters are responsible for the output uncertainty, three sensitivity methods (Standardized Regression Coefficients, Morris and differential analysis) were evaluated and compared. The results from these methods were mostly in agreement with each other and revealed that only few parameters (about 10) out of a total 56 were mainly responsible for the output uncertainty. Among these significant parameters, one finds parameters related to fermentation characteristics such as biomass metabolism, chemical equilibria and mass-transfer. Overall the uncertainty and sensitivity analysis are found promising for helping to build reliable mechanistic models and to interpret the model outputs properly. These tools make part of good modeling practice, which can contribute to successful PAT applications for increased process understanding, operation and control purposes. © 2009 American Institute of Chemical Engineers Biotechnol. Prog., 2009

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Microbial Biotechnology, Department of Systems Biology
Contributors: Sin, G., Gernaey, K., Eliasson Lantz, A.
Pages: 1043-1053
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Biotechnology Progress
Volume: 25
Issue number: 4
ISSN (Print): 8756-7938
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.12 SJR 0.676 SNIP 0.785
Web of Science (2017): Impact factor 1.947
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.12 SJR 0.699 SNIP 0.768
Web of Science (2016): Impact factor 1.986
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.07 SJR 0.729 SNIP 0.805
Web of Science (2015): Impact factor 2.167
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.2 SJR 0.812 SNIP 0.929
Web of Science (2014): Impact factor 2.149
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.16 SJR 0.768 SNIP 0.857
Web of Science (2013): Impact factor 1.883
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.35 SJR 0.831 SNIP 0.871
Web of Science (2012): Impact factor 1.853
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.4 SJR 0.917 SNIP 0.948
Web of Science (2011): Impact factor 2.34
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.997 SNIP 0.934
Web of Science (2010): Impact factor 2.178
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.969 SNIP 1.038
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.895 SNIP 0.987
Scopus rating (2007): SJR 1.02 SNIP 1.083
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.977 SNIP 1.104
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.911 SNIP 1.022
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.727 SNIP 0.955
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.74 SNIP 0.945
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.867 SNIP 1.069
Improving the Morris method for sensitivity analysis by scaling the elementary effects

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Sin, G., Gernaey, K.
Publication date: 2009

Event information
Event: 19th European Symposium on Computer Aided Process Engineering – ESCAPE19
Location: Krakow, Poland
Source: orbit
Source-ID: 248216
Research output: Research › Sound/Visual production (digital) – Annual report year: 2009

Introducing mechanistic models in Process Analytical Technology education

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Gernaey, K., Woodley, J., Sin, G.
Pages: 593-598
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Biotechnology Journal
Volume: 4
Issue number: 5
ISSN (Print): 1860-6768
Lægemiddelproduktion - brugen af modellering og PAT

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Microbial Biotechnology, Department of Systems Biology, CHEC Research Centre
Contributors: Gernaey, K., Sin, G., Eliasson Lantz, A., Woodley, J., Gani, R., Dam-Johansen, K.
Pages: 22-24
Publication date: 2009
Mechanistic models and advanced model analysis within a PAT framework

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Center for Microbial Biotechnology, Department of Systems Biology, Computer Aided Process Engineering Center
Contributors: Gernaey, K., Woodley, J., Eliasson Lantz, A., Sin, G.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 14th European Congress on Biotechnology, Barcelona, Spain.
Source: orbit
Source-ID: 255677
Research output: Research - peer-review › Poster – Annual report year: 2009

Modelling, Simulation and Optimization of Single-Cell Protein Production in a U-Loop Reactor

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Publication date: 2009
Event information
Event: 2009 AIChE Annual Meeting
Location: Nashville, TN, United States
Source: orbit
Source-ID: 252816
Research output: Research › Sound/Visual production (digital) – Annual report year: 2009

Multi-criteria decision making under uncertainty: Energy efficient and low-carbon wastewater treatment (keynote lecture)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Sin, G.
Publication date: 2009
Event information
Event: 5th Dubrovnik Conference on Sustainable Development of Energy, Water and Environment Systems
Location: Dubrovnik, Croatia
Source: orbit
Source-ID: 250770
Research output: Research › Sound/Visual production (digital) – Annual report year: 2009
Systematic framework for modeling multi-enzymatic synthetic processes

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Andrade Santacoloma, P. D. G., Sin, G., Gernaey, K., Woodley, J.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at Biotrans 09, Bern, Switzerland.
Source: orbit
Source-ID: 255602

Systematic model development for partial nitrification of landfill leachate in a SBR

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: Ganigué, R., Volcke, E., Puig, S., Balaguer, M., Colprim, J., Sin, G.
Publication date: 2009

Event
Event: 2nd IWA Specialized Conference on nutrient management in wastewater treatment
Location: Krakow, Poland, 6-9 September
Source: orbit
Source-ID: 249749

Uncertainty analysis in WWTP model applications: a critical discussion using an example from design
This study focuses on uncertainty analysis of WWTP models and analyzes the issue of framing and how it affects the interpretation of uncertainty analysis results. As a case study, the prediction of uncertainty involved in model-based design of a wastewater treatment plant is studied. The Monte Carlo procedure is used for uncertainty estimation, for which the input uncertainty is quantified through expert elicitation and the sampling is performed using the Latin hypercube method. Three scenarios from engineering practice are selected to examine the issue of framing: (1) uncertainty due to stoichiometric, biokinetic and influent parameters; (2) uncertainty due to hydraulic behaviour of the plant and mass transfer parameters; (3) uncertainty due to the combination of (1) and (2). The results demonstrate that depending on the way the uncertainty analysis is framed, the estimated uncertainty of design performance criteria differs significantly. The implication for the practical applications of uncertainty analysis in the wastewater industry is profound: (i) as the uncertainty analysis results are specific to the framing used, the results must be interpreted within the context of that framing; and (ii) the framing must be crafted according to the particular purpose of uncertainty analysis/model application. Finally, it needs to be emphasised that uncertainty analysis is no doubt a powerful tool for model-based design among others, however clear guidelines for good uncertainty analysis in wastewater engineering practice are needed.

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Sin, G., Gernaey, K., Neumann, M. B., Loosdrecht, M. C. V., Gujer, W.
Pages: 2894-2906
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Water Research
Volume: 43
Issue number: 11
ISSN (Print): 0043-1354
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.358
Web of Science (2017): Impact factor 7.051
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.49 SJR 2.663 SNIP 2.563
Web of Science (2016): Impact factor 6.942
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.63 SJR 2.665 SNIP 2.482
Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.13 SJR 2.946 SNIP 2.702
Web of Science (2014): Impact factor 5.528
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.02 SJR 2.956 SNIP 2.676
Web of Science (2013): Impact factor 5.323
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.15 SJR 2.914 SNIP 2.442
Web of Science (2012): Impact factor 4.655
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.43 SJR 2.862 SNIP 2.355
Web of Science (2011): Impact factor 4.865
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.592 SNIP 2.192
Web of Science (2010): Impact factor 4.546
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.319 SNIP 2.224
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.073 SNIP 2.178
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.94 SNIP 2.184
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.902 SNIP 2.233
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.113 SNIP 2.334
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.209 SNIP 2.108
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.702 SNIP 1.908
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.568 SNIP 1.757
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.319 SNIP 1.69
Uncertainty and sensitivity analysis of control strategies using the benchmark simulation model No1 (BSM1)

The objective of this paper is to perform an uncertainty and sensitivity analysis of the predictions of the Benchmark Simulation Model (BSM) No. 1, when comparing four activated sludge control strategies. The Monte Carlo simulation technique is used to evaluate the uncertainty in the BSM1 predictions, considering the ASM1 bio-kinetic parameters and influent fractions as input uncertainties while the Effluent Quality Index (EQI) and the Operating Cost Index (OCI) are focused on as model outputs. The resulting Monte Carlo simulations are presented using descriptive statistics indicating the degree of uncertainty in the predicted EQI and OCI. Next, the Standard Regression Coefficients (SRC) method is used for sensitivity analysis to identify which input parameters influence the uncertainty in the EQI predictions the most. The results show that control strategies including an ammonium (S-NH) controller reduce uncertainty in both overall pollution removal and effluent total Kjeldahl nitrogen. Also, control strategies with an external carbon source reduce the effluent nitrate (S-NO) uncertainty increasing both their economical cost and variability as a trade-off. Finally, the maximum specific autotrophic growth rate (μ(A)) causes most of the variance in the effluent for all the evaluated control strategies. The influence of denitrification related parameters, e. g. eta(g) (anoxic growth rate correction factor) and eta(h) (anoxic hydrolysis rate correction factor), becomes less important when a S-NO controller manipulating an external carbon source addition is implemented.

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Flores-Alsina, X., Rodriguez-Roda, I., Sin, G., Gernaey, K.
Pages: 491-499
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Water Science and Technology
Volume: 59
Issue number: 3
ISSN (Print): 0273-1223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
Wastewater treatment modelling: dealing with uncertainties

This paper serves as a problem statement of the issues surrounding uncertainty in wastewater treatment modelling. The paper proposes a structure for identifying the sources of uncertainty introduced during each step of an engineering project concerned with model-based design or optimisation of a wastewater treatment system. It briefly references the methods currently used to evaluate prediction accuracy and uncertainty and discusses the relevance of uncertainty evaluations in model applications. The paper aims to raise awareness and initiate a comprehensive discussion among professionals on
model prediction accuracy and uncertainty issues. It also aims to identify future research needs. Ultimately the goal of such a discussion would be to generate transparent and objective methods of explicitly evaluating the reliability of model results, before they are implemented in an engineering decision-making context.

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Pages: 1929-1941
Publication date: 2009
Peer-reviewed: Yes

**Publication information**
Journal: Water Science and Technology
Volume: 60
Issue number: 8
ISSN (Print): 0273-1223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Web of Science (2012): Impact factor 1.102
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.25 SJR 0.594 SNIP 0.631
Web of Science (2011): Impact factor 1.122
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.529 SNIP 0.597
Web of Science (2010): Impact factor 1.056
Web of Science (2010): Indexed yes
An efficient approach to automate the manual trial and error calibration of activated sludge models

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Ghent University, DA Drogisterij, Universite Laval
Contributors: Sin, G., Pauw, D. J. D., Weijers, S., Vanrolleghem, P. A.
Pages: 516-528
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Biotechnology and Bioengineering (Print)
Volume: 100
Issue number: 3
ISSN (Print): 0006-3592
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.07 SJR 1.372 SNIP 1.186
Web of Science (2017): Impact factor 3.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.447 SNIP 1.178
Web of Science (2016): Impact factor 4.481
Web of Science (2016): Indexed yes
Application of mechanistic models within a PAT framework

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Contributors: Gernaey, K., Sin, G., Albo, E., Woodley, J., Singh, R., Gani, R.
Publication date: 2008

Event information
Event: ISPE conference
Location: Malmö, Sweden
Source: orbit
Source-ID: 231446
Research output: Research - Sound/Visual production (digital) – Annual report year: 2008

Combining Multiway Principal Component Analysis (MPCA) and clustering for efficient data mining of historical data sets of SBR processes

A methodology based on Principal Component Analysis (PCA) and clustering is evaluated for process monitoring and process analysis of a pilot-scale SBR removing nitrogen and phosphorus. The first step of this method is to build a multi-way PCA (MPCA) model using the historical process data. In the second step, the principal scores and the Q-statistics resulting from the MPCA model are fed to the LAMDA clustering algorithm. This procedure is iterated twice. The first iteration provides an efficient and effective discrimination between normal and abnormal operational conditions. The second iteration of the procedure allowed a clear-cut discrimination of applied operational changes in the SBR history. Important to add is that this procedure helped identifying some changes in the process behaviour, which would not have been possible, had we only relied on visually inspecting this online data set of the SBR (which is traditionally the case in practice). Hence the PCA based clustering methodology is a promising tool to efficiently interpret and analyse the SBR process behaviour using large historical online data sets.

General information
State: Published
Organisations: University of Girona, Lund University, Ghent University
Contributors: Villiez, K., Sin, G., Vanrolleghem, P. A., Ruiz, M., Colomer, J., Rosén, C.
Pages: 1659-1666
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Water Science and Technology
Volume: 57
Issue number: 10
ISSN (Print): 0273-1223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
Developing a framework for continuous use of models in daily management and operation of WWTPs: A life cycle approach

We developed and evaluated a framework for the continuous use of dynamic models in daily management and operation of WWTPs. The overall aim is to generate knowledge and build in-house capacity for the reliable use of dynamic models in practice (within a regional water authority in The Netherlands). To this end, we have adopted a life cycle approach, where the plant model follows the different stages that make up the typical lifespan of a plant. Since this approach creates a framework in which models are continuously reused, it is more efficient in terms of resources and investment than the traditional approach where one always makes a new model for the plant whenever it is needed. The methodology was evaluated successfully at a 50,000 PE domestic EBPR plant (Haaren, The Netherlands). It is shown that the continuous use and update of models in a cyclic manner creates a learning cycle, which results in experience and knowledge generation about the plant's modelling that accumulates and translates into improvements into the modelling quality and efficiency. Moreover, a model is now always on-the-shelf for process optimization.

General information
State: Published
Organisations: Ghent University
Contributors: Sin, G., de Pauw, D., Weijers, S., Vanrolleghem, P.
Pages: 1301-1307
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Water Science and Technology
Volume: 57
Issue number: 9
ISSN (Print): 0273-1223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Web of Science (2012): Impact factor 1.102
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.25 SJR 0.594 SNIP 0.631
Web of Science (2011): Impact factor 1.122
Dynamic model development and validation for a nitrifying moving bed biofilter: Effect of temperature and influent load on the performance

A mathematical model with adequate complexity integrating hydraulics, biofilm and microbial conversion processes is successfully developed for a continuously moving bed biofilter performing tertiary nitrification. The model was calibrated and validated using data from Nether Stowey pilot plant in UK. For the model, the mixing is approximated using tanks-in-series approach, the biofilm is described using a one-dimensional multi-species model, and the microbial processes are described by ASM1. A scenario analysis with the model revealed that the temperature has a significant impact on the ammonium removal efficiency, doubling nitrification capacity every 5 degrees C increase. However, at temperatures higher than 20 degrees C, the biofilm thickness starts to decrease due to increased decay rate. The influent nitrogen load was also found to be influential on the filter performance, while the hydraulic loading had relatively negligible impact. Overall, the calibrated model can now reliably be used for design and process optimization purposes.

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Ghent University
Contributors: Sin, G., Weijma, J., Spanjers, H., Nopens, I.
Pages: 384-397
Publication date: 2008
Peer-reviewed: Yes
Evaluating prediction uncertainty of fermentation models

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Center for Microbial Biotechnology, Department of Systems Biology
Contributors: Sin, G., Eliasson Lantz, A., Gernaey, K.
Publication date: 2008

Event information
Event: 7th European Symposium on Biochemical Engineering Science
Location: Faro, Portugal
Source: orbit
Source-ID: 229396
Research output: Research › Sound/Visual production (digital) – Annual report year: 2008

Matrix Notation for Efficient Development of First-Principles Models Within PAT Applications: Integrated Modeling of Antibiotic Production With Streptomyces coelicolor

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Center for Microbial Biotechnology, Department of Systems Biology
Contributors: Sin, G., Ödman, P., Petersen, N., Eliasson Lantz, A., Gernaey, K.
Pages: 153-171
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Biotechnology and Bioengineering (Print)
Volume: 101
ISSN (Print): 0006-3592
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.07 SJR 1.372 SNIP 1.186
Web of Science (2017): Impact factor 3.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.447 SNIP 1.178
Web of Science (2016): Impact factor 4.481
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Mechanistic models for evaluation of alternative fermentation control strategies within a PAT framework

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Contributors: Gernaey, K., Albo, E., Woodley, J., Sin, G.
Publication date: 2008

Event information
Event: 7th European Symposium on Biochemical Engineering Science
Location: Faro, Portugal
Source: orbit
Source-ID: 223690

Modelling nitrite in wastewater treatment systems: A discussion of different modelling concepts

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Pages: 1155-1171
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Water Science and Technology
Volume: 58
Issue number: 6
ISSN (Print): 0273-1223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Multi-criteria evaluation of wastewater treatment plant control strategies under uncertainty

The evaluation of activated sludge control strategies in wastewater treatment plants (WWTP) via mathematical modelling is a complex activity because several objectives; e.g. economic, environmental, technical and legal; must be taken into account at the same time, i.e. the evaluation of the alternatives is a multi-criteria problem. Activated sludge models are not well characterized and some of the parameters can present uncertainty, e.g. the influent fractions arriving to the facility and the effect of either temperature or toxic compounds on the kinetic parameters, having a strong influence in the model predictions used during the evaluation of the alternatives and affecting the resulting rank of preferences. Using a simplified version of the IWA Benchmark Simulation Model No. 2 as a case study, this article shows the variations in the decision making when the uncertainty in activated sludge model (ASM) parameters is either included or not during the evaluation of WWTP control strategies. This paper comprises two main sections. Firstly, there is the evaluation of six WWTP control strategies using multi-criteria decision analysis setting the ASM parameters at their default value. In the following section, the uncertainty is introduced, i.e. input uncertainty, which is characterized by probability distribution functions based on the available process knowledge. Next, Monte Carlo simulations are run to propagate input through the model and affect the different outcomes. Thus (i) the variation in the overall degree of satisfaction of the control objectives for the generated
WWTP control strategies is quantified, (ii) the contributions of environmental, legal, technical and economic objectives to the existing variance are identified and finally (iii) the influence of the relative importance of the control objectives during the selection of alternatives is analyzed. The results show that the control strategies with an external carbon source reduce the output uncertainty in the criteria used to quantify the degree of satisfaction of environmental, technical and legal objectives, but increasing the economical costs and their variability as a trade-off. Also, it is shown how a preliminary selected alternative with cascade ammonium controller becomes less desirable when input uncertainty is included, having simpler alternatives more chance of success. (C) 2008 Elsevier Ltd. All rights reserved.
Nitrite effect on the phosphorus uptake activity of phosphate accumulating organisms (PAOs) in pilot-scale SBR and MBR reactors

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, University College West Flanders, Ghent University, Universite Laval
Contributors: Sin, G., Niville, K., Bachis, G., Jiang, T., Nopens, I., van Hulle, S., Vanrolleghem, P. A.
Pages: 249-260
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Water SA (Online Edition)
Volume: 34
Issue number: 2
ISSN (Print): 0378-4738
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.06 SJR 0.361 SNIP 0.624
Web of Science (2017): Impact factor 0.783
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Practical identifiability of complex fermentation models: a systematic approach

**General information**
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Sin, G., Gernaey, K.
Publication date: 2008
Uncertainty analysis in WWTP model applications: a critical discussion of issues using a design example

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Sin, G., Gernaey, K., Neumann, M., van Loosdrecht, M. C., Gujer, W.
Publication date: 2008

Event information
Event: 7th European Symposium on Biochemical Engineering Science
Location: Faro, Portugal
Source: orbit
Source-ID: 229397
Research output: Research › Sound/Visual production (digital) – Annual report year: 2008

Uncertainty and sensitivity analysis of control strategies using the benchmark simulation model no 1 (BSM1)

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Flores Alsina, X., Sin, G., Rodríguez-Roda, I., Gernaey, K.
Pages: 1331-1338
Publication date: 2008

Host publication information
Title of host publication: Proceedings of the iEMSs Fourth Biennial Meeting: International Congress on Environmental Modelling and Software (iEMSs 2008)
Publisher: Universitat Politècnica de Catalunya
Editors: Sànchez-Marrè, M., Béjar, J., Comas, J., Rizzoli, A. E., Guariso, G.
ISBN (Print): 978-84-7653-074-0
Source: orbit
Source-ID: 229412
Research output: Research - peer-review › Article in proceedings – Annual report year: 2008

Wastewater Treatment Models
The state-of-the-art level reached in modeling wastewater treatment plants (WWTPs) is reported. For suspended growth systems, WWTP models have evolved from simple description of biological removal of organic carbon and nitrogen in aeration tanks (ASM1 in 1987) to more advanced levels including description of biological phosphorus removal, physical-chemical processes, hydraulics, and settling tanks. For attached growth systems, biofilm models have progressed from analytical steady-state models to more complex 2-D/3-D dynamic numerical models. Plant-wide modeling is set to advance further the practice of WWTP modeling by linking the wastewater treatment line with the sludge handling line in one modeling platform. Application of WWTP models is currently rather time consuming and thus expensive due to the high model complexity, and requires a great deal of process knowledge and modeling expertise. Efficient and good modeling practice therefore requires the use of a proper set of guidelines, thus grounding the modeling studies on a general and systematic framework. Last but not least, general limitations of WWTP models – more specifically, activated sludge models – are introduced since these define a boundary of validity for WWTP model applications.

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Gernaey, K., Sin, G.
Pages: 3705-3718
Publication date: 2008

Host publication information
Title of host publication: Encyclopedia of Ecology
Volume: Vol. 5: Ecological Models
Experimental data quality and quantity influence on parameter estimation accuracy: Andrews inhibition model as a case study

General information
State: Published
Organisations: Autonomous University of Barcelona, Ghent University
Contributors: Guisasola, A., Baeza, J., Carrera, J., Sin, G., Vanrolleghem, P., Lafuente, J.
Pages: 139-145
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Education for Chemical Engineers
Volume: 1
Original language: English
Source: orbit
Source-ID: 244992
Research output: Research - peer-review › Book chapter – Annual report year: 2008

Extensions to modeling aerobic carbon degradation using combined respirometric–titrimetric measurements in view of activated sludge model calibration

General information
State: Published
Organisations: Universite Laval, Ghent University
Contributors: Sin, G., Vanrolleghem, P. A.
Pages: 3345-2258
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Water Research
Volume: 41
Issue number: 15
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.358
Web of Science (2017): Impact factor 7.051
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.49 SJR 2.663 SNIP 2.563
Web of Science (2016): Impact factor 6.942
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.63 SJR 2.665 SNIP 2.482
Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Modellering van rioolwaterzuiveringsinstallaties

General information
State: Published
Parameter subset selection for the dynamic calibration of activated sludge models (ASMs): experience versus systems analysis

In this work we address the issue of parameter subset selection within the scope of activated sludge model calibration. To this end, we evaluate two approaches: (i) systems analysis and (ii) experience-based approach. The evaluation has been carried out using a dynamic model (ASM2d) calibrated to describe nitrogen and phosphorus removal in the Haaren WWTP (The Netherlands). The parameter significance ranking shows that the temperature correction coefficients are among the most influential parameters on the model output. This outcome confronts the previous identifiability studies and the experience based approaches which excluded them from their analysis. Systems analysis reveals that parameter significance ranking and size of the identifiable parameter subset depend on the information content of data available for calibration. However, it suffers from heavy computational demand. In contrast, although the experience-based approach is computationally affordable, it is unable to take into account the information content issue and therefore can be either too optimistic (giving poorly identifiable sets) or pessimistic (small size of sets while much more can be estimated from the data). An appropriate combinations of both approaches is proposed which offers a realistic (doable) and sound approach for parameter subset selection in activated sludge modelling.
A calibration methodology and model-based systems analysis for SBRs removing nutrients under limited aeration conditions

A methodology is proposed for the model calibration of nutrient-removing laboratory-scale SBRs under limited aeration. Based on in-process measurements and influent wastewater characterization, the ASM2d model was modified by adding
an organic nitrogen module incorporating a hydrolysis mechanism. After calibration, the simulation results showed that enhanced biological nutrient removal occurred during the fill period and under reduced aeration achieving so-called 'simultaneous nutrient removal'. A model-based systems analysis was performed in terms of the contributions of different processes to overall oxygen, nitrogen and phosphate utilization. In each phase, simultaneously occurring biological reactions were compared using the calibrated model. According to the calibrated model, 61% of all denitrified nitrate is denitrified during the mixing/filling phase. On the other hand, 17% of all denitrified nitrate is consumed by simultaneous nitrification-denitrification during the first aerobic period. The aerobic and anoxic P-removals were quantified as 73% and 12%, respectively. (c) 2006 Society of Chemical Industry.
Application of a model-based optimisation methodology for nutrient removing SBRs leads to falsification of the model

Recently, a model-based optimisation methodology for SBR operation has been developed and an optimal operation scenario proposed to improve N and P removal in a pilot-scale SBR. In this study, this optimal operation scenario was implemented and evaluated. The results of the implementation showed that the SBR performance was improved by approximately 50 and 40% for total nitrogen and phosphorous removal, respectively, which was better than predicted by the model. However, the long-term SBR performance was found to be unstable, particularly owing to settling problems developed after the implementation. When confronted with reality, the model used for the optimisation of the operation was found to be invalid. The model was unable to predict the nitrite build-up provoked by the optimal operation scenario. These results imply that changing the operation of an SBR system using a model may significantly change the behaviour of the system beyond the (unknown) application domain of the model. This is simply because the mechanistic models currently do not cover all the aspects of activated sludge systems, e.g. settling and adaptation of the microbial community. To further improve model-application practices, expert knowledge (not contained in the models) can be valuable and should be incorporated into model-based process optimisations.

General information
State: Published
Organisations: Ghent University
Contributors: Sin, G., Villez, K., Vanrolleghem, P.
Pages: 95-103
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Water Science and Technology
Volume: 53
Issue number: 4-5
ISSN (Print): 0273-1223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Web of Science (2012): Impact factor 1.102
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.25 SJR 0.594 SNIP 0.631
Web of Science (2011): Impact factor 1.122
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.529 SNIP 0.597
Web of Science (2010): Impact factor 1.056
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.592 SNIP 0.693
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.583 SNIP 0.694
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.736 SNIP 0.766
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.696 SNIP 0.789
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.767 SNIP 0.841
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.875 SNIP 0.897
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.882 SNIP 0.897
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.877 SNIP 0.894
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.758 SNIP 0.967
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.887 SNIP 0.866
Web of Science (2000): Indexed yes
Evaluation of the impacts of model-based operation of SBRs on activated sludge microbial community
Impact of model-based operation of nutrient removing SBRs on the stability of activated sludge population was studied in this contribution. The optimal operation scenario found by the systematic model-based optimisation protocol of Sin et al. (Wat. Sci. Tech., 2004, 50(10), 97-105) was applied to a pilotscale SBR and observed to considerably improve the nutrient removal efficiency in the system. Further, the process dynamics was observed to change under the optimal operation scenario, e.g. the nitrite route prevailed and also filamentous bulking was provoked in the SBR system. At the microbial community level as monitored by DGGE, a transient shift was observed to gradually take place parallel to the shift into the optimal operation scenario. This implies that the model-based optimisation of a nutrient removing SBR causes changes at the, microbial community level: This opens future perspectives to incorporate the valuable information from the molecular monitoring of activated sludge into the model-based optimisation methodologies. In this way, it is expected that model-based optimisation approaches will better cover complex and dynamic aspects of activated sludge systems.

General information
State: Published
Organisations: Ghent University
Contributors: Sin, G., Goyoreanu, R., Boon, N., Schelstraete, G., Vanrolleghem, P.
Pages: 157-166
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Water Science and Technology
Volume: 54
Issue number: 1
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Evolution of an ASM2d-like model structure due to operational changes of an SBR process

To model biological nitrogen and phosphorus removal systems with an affordable complexity, the ASM2d model structure is based on many assumptions. In this study, some of these assumptions, however, were observed to become invalid when the biological behaviour in the system altered in response to changes in the operation of the system, a pilot-scale N and P removing SBR. Particularly, the three applied operational scenarios resulted in three distinctive responses in the SBR, namely pronounced limitation of the hydrolysis of the organic nitrogen, nitrite build-up during aerobic conditions and also nitrite build-up during anoxic conditions. This shows that even for the same system with the same influent wastewater composition, the model structure of the ASM2d does not remain constant but adapts parallel to dynamic changes in the activated sludge community. On the other hand, the three calibrated ASM2d models still lacked the ability to entirely describe the observed dynamics particularly those dealing with the phosphorus dynamics and hydrolysis. Understanding the underlying reasons of this discrepancy is a challenging task, which is expected to improve the modelling of bio-P removing activated sludge systems.

General information
State: Published
Model-based evaluation of an on-line control strategy for SBRs based on OUR and ORP measurements

Application of control strategies for existing wastewater treatment technologies becomes necessary to meet ever-stricter effluent legislations and reduce the associated treatment costs. In the case of SBR technology, controlling the phase scheduling is one of the key aspects of SBR operation. In this study a calibrated mechanistic model based on the ASM1 was used to evaluate an on-line control strategy for the SBR phase-scheduling and compare it with the SBR's performance using no control strategy. To evaluate the performance, reference indices relating to the effluent quality, the required energy for aeration and the treated wastewater volume were used. The results showed that it is possible to maintain optimal SBR performance in the studied system at minimal costs by on-line control of the length of the aerobic and anoxic phases.

General information
State: Published
Organisations: University of Girona, Ghent University
Contributors: Corominas, L., Sin, G., Puig, S., Traore, A., Balaguera, M., Colprim, J., Vanrolleghem, P.
Pages: 161-169
Publication date: 2006
Peer-reviewed: Yes

Publication information
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Web of Science (2012): Impact factor 1.102
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.25 SJR 0.594 SNIP 0.631
Web of Science (2011): Impact factor 1.122
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.529 SNIP 0.597
Web of Science (2010): Impact factor 1.056
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.592 SNIP 0.693
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.583 SNIP 0.694
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.736 SNIP 0.766
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.696 SNIP 0.789
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.767 SNIP 0.841
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.875 SNIP 0.897
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.882 SNIP 0.897
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.877 SNIP 0.894
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.758 SNIP 0.967
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.887 SNIP 0.866
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.885 SNIP 0.91
Original language: English
DOIs:
10.2166/wst.2006.120
Simple modification to describe the soil water retention curve between saturation and oven dryness

Prediction of water and vapor flow in porous media requires an accurate estimation of the soil water retention curve describing the relation between matric potential and the respective soil water content from saturation to oven dryness. In this study, we modified the Kosugi (1999) function to represent soil water retention at all matric potentials. This modification retains the form of the original Kosugi function in the wet range and transforms to an adsorption equation in the dry range. Following a systems identification approach, the extended function was tested against observed data taken from literature that cover the complete range of water contents from saturation to almost oven dryness with textures ranging from sand to silty clay. The uncertainty of parameter estimates (confidence intervals) as well as the correlation between parameters was studied. The predictive capability of the extended model was evaluated under two reduced sets of data that do not contain observations below a matric potential of -1500 and -100 kPa. This evaluation showed that the extended model successfully predicted the water content with acceptable uncertainty. These results add confidence into the proposed modification and suggest that it can be used to better predict the soil water retention curve, particularly under reduced data sets.

General information
State: Published
Organisations: Ghent University
Contributors: Khlosi, M., Cornelis, W., Gabriels, D., Sin, G.
Pages: W11501
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Water Resources Research
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ISSN (Print): 0043-1397
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.39 SJR 2.296 SNIP 1.555
Web of Science (2017): Impact factor 4.361
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.1 SJR 2.615 SNIP 1.633
Web of Science (2016): Impact factor 4.397
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.06 SJR 2.525 SNIP 1.593
Web of Science (2015): Impact factor 3.792
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.75 SJR 2.442 SNIP 1.668
Web of Science (2014): Impact factor 3.549
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.65 SJR 2.204 SNIP 1.751
Web of Science (2013): Impact factor 3.709
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.12 SJR 2.127 SNIP 1.586
Web of Science (2012): Impact factor 3.149
ISI indexed (2012): ISI indexed yes
A critical comparison of systematic calibration protocols for activated sludge models: A SWOT analysis

Modelling activated sludge systems has gained an increasing momentum after the introduction of activated sludge models (ASMs) in 1987. Application of dynamic models for full-scale systems requires essentially a calibration of the chosen ASM to the case under study. Numerous full-scale model applications have been performed so far which were mostly based on ad hoc approaches and expert knowledge. Further, each modelling study has followed a different calibration approach: e.g. different influent wastewater characterization methods, different kinetic parameter estimation methods, different selection of parameters to be calibrated, different priorities within the calibration steps, etc. In short, there was no standard approach in performing the calibration study, which makes it difficult, if not impossible, to (1) compare different calibrations of ASMs with each other and (2) perform internal quality checks for each calibration study. To address these concerns, systematic calibration protocols have recently been proposed to bring guidance to the modeling of activated sludge systems and in particular to the calibration of full-scale models. In this contribution four existing calibration approaches (BIOMATH, HSG, STOWA and WERF) will be critically discussed using a SWOT (Strengths, Weaknesses, Opportunities, Threats) analysis. It will also be assessed in what way these approaches can be further developed in view of further improving the quality of ASM calibration. In this respect, the potential of automating some steps of the calibration procedure by use of mathematical algorithms is highlighted. (c) 2005 Elsevier Ltd. All rights reserved.
A new approach for modelling simultaneous storage and growth processes for activated sludge systems under aerobic conditions

By critically evaluating previous models, a new mechanistic model is developed to describe simultaneous storage and growth processes occurring in activated sludge systems under aerobic conditions. Identifiability was considered an important criterion during the model development since it among others helps to increase the reliability and applicability of models to full-scale WWTPs. A second order model was proposed for description of the degradation of the storage products under famine conditions. The model is successfully calibrated by only using OUR data obtained from batch experiments. Calibrations were performed with biomass from full-scale WWTPs in Belgium and Spain. Predictions of the calibrated model were successfully confirmed using off-line PHB measurements, supporting the validity of the model. An iterative experimental design procedure was successfully applied and found to remarkably improve the parameter estimation accuracy for the growth on storage parameters K-1 and K-2, which used to have large confidence intervals when using standard experiments. The estimated biomass growth yield on substrate (0.58 mgCOD/mgCOD) is quite close to the theoretically expected range for heterotrophic growth. This became possible by properly accounting for the storage process. Moreover, the maximum growth rate was predicted in the range 0.7-1.3 per day. This range, albeit quite lower than the values reported for the growth-based ASM models, is believed to be more realistic. Finally, the new model is expected to better and more mechanistically describe simultaneous storage and growth activities of activated sludge systems and as such could contribute to improved design, operation and control of those systems. (c) 2005 Wiley Periodicals, Inc.
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.447 SNIP 1.178
Web of Science (2016): Impact factor 4.481
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.44 SJR 1.632 SNIP 1.355
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.16 SJR 1.612 SNIP 1.395
Web of Science (2014): Impact factor 4.126
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.4 SJR 1.637 SNIP 1.427
Web of Science (2013): Impact factor 4.164
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.04 SJR 1.62 SNIP 1.364
Web of Science (2012): Impact factor 3.648
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.08 SJR 1.668 SNIP 1.481
Web of Science (2011): Impact factor 3.946
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.551 SNIP 1.354
Web of Science (2010): Impact factor 3.7
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.498 SNIP 1.358
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.248 SNIP 1.283
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.363 SNIP 1.356
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.467 SNIP 1.437
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.135 SNIP 1.23
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.105 SNIP 1.245
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.052 SNIP 1.228
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.117 SNIP 1.263
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.059 SNIP 1.16
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.428 SNIP 1.529
Web of Science (2000): Indexed yes
Limitations of ASM1 and ASM3: A comparison based on batch oxygen uptake rate profiles from different CD full-scale wastewater treatment plants

The two most popular models for the description of the biological COD removal are ASM1 and ASM3. However, some numerical inconsistencies arise when using these models to interpret the data obtained in short-term respirometric batch experiments. In this study, both models are fitted to four different respirometric batch profiles obtained with biomass from different WWTP. The parameter estimation results and the practical (local) identifiability are analysed, and the limitations of both models are discussed. The growth yield obtained by fitting ASM1 to the short-term respirometric batch profiles is higher than the default one, as well as the storage yield obtained by fitting ASM3 is lower than the default one. Based on these values, possible improvements to the modelling of the biological COD removal, such as the inclusion of simultaneous growth and storage on external substrate, are proposed.
A nitrate biosensor based methodology for monitoring anoxic activated sludge activity

An improved methodology based on a nitrate biosensor is developed and applied successfully for in-depth monitoring and study of anoxic activated sludge activities. The major advantages of the methodology are its simplicity, reliability and high data quality. The resulting data allowed for the first time to monitor anoxic respiration rate of activated sludge (nitrate uptake rate (NUR)) at a high time resolution making it clearly comparable with high frequency oxygen uptake rate (OUR) measurements obtained under aerobic conditions. Further, the anoxic respiration data resulting from a pulse addition of carbon source to endogenously respiring anoxic activated sludge shows a clear start-up phenomenon and storage tail that is usually also observed in high-frequency OUR measurements. Finally, the improved methodology can be expected to serve as an anoxic respirometer for activated sludge treatment plants where denitrification process occurs in single-step. Further, it can be used for a variety of purposes e.g. for toxicity and activity monitoring, process control and parameter estimation of the activated sludge process, similar to the aerobic respirometers.

General information
State: Published
Organisations: Ghent University
Contributors: Sin, G., Vanrolleghem, P.
Pages: 125-133
Modeling off a large-scale wastewater treatment plant for efficient operation

Environmental legislations in the Western world impose stringent effluent quality standards for ultimate protection of the environment. This is also observed in Turkey. The current paper presents efforts made to simulate an existing 0.77 million m$^3$/day conventional activated sludge plant located at Ankara, AWTP. The ASM1 model was used for simulation in this study. The model contains numerous stoichiometric and kinetic parameters, some of which need to be determined on case by case bases. The easily degradable COD (SS) was determined by two methods, physical-chemical and respirometric methods, namely. The latter method was deemed unreliable and rejected in the further study. Dynamic simulation with SSSP program predicted effluent COD and MLSS values successfully while overestimating OUR. A complete fit could only be obtained by introducing a dimensionless correction factor ($\eta(O_2)=0.58$) to the oxygen term in ASM1.

General information
State: Published
Organisations: Middle East Technical University (METU)
Contributors: Gökçay, C., Sin, G.
Pages: 123-130
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Peer-reviewed: Yes

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Journal: Water Science and Technology
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BFI (2018): BFI-level 1
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Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
Optimal but robust N and P removal in SBRs: a model-based systematic study of operation scenarios

A systematic approach to determine the optimal operation strategy for nitrogen (N) and phosphorus (P) removal of sequencing batch reactors (SBRs) has been developed and applied successfully to a lab-scale SBR. The methodology developed is based on using a grid of possible scenarios to simulate the effect of the key degrees of freedom in the SBR.
system. The grid of scenarios is simulated using a calibrated ASM2dN model developed and calibrated in a previous study. Effluent quality in combination with a robustness index for each of the scenarios is used to select the best scenario. With the best scenario, it is possible to improve/increase the current performance of the SBR system by around 54% and 74% for N and P removal respectively.

**General information**

State: Published
Organisations: Ghent University
Contributors: Sin, G., Insel, G., Lee, D., Vanrolleghem, P.
Pages: 97-105
Publication date: 2004
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**Publication information**

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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.19 SJR 0.464 SNIP 0.594
Web of Science (2015): Impact factor 1.064
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.14 SJR 0.585 SNIP 0.683
Web of Science (2014): Impact factor 1.106
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.3 SJR 0.571 SNIP 0.701
Web of Science (2013): Impact factor 1.212
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.13 SJR 0.597 SNIP 0.659
Web of Science (2012): Impact factor 1.102
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.25 SJR 0.594 SNIP 0.631
Web of Science (2011): Impact factor 1.122
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.529 SNIP 0.597
Web of Science (2010): Impact factor 1.056
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.592 SNIP 0.693
An integrated sensor for the monitoring of aerobic and anoxic activated sludge activities in biological nitrogen removal plants

An integrated sensor is developed as a tool for monitoring the activated sludge activity on which the performance of the treatment plant depends. The sensor provides information-rich data of high frequency obtained from respirometric-titrimetric and nitrate measurements in one single set-up. The sensor is shown to successfully monitor and provide in-depth insight into nitrification, denitrification and carbon source degradation processes occurring in BNR plants. Based on the experimental results it is hypothesized that the ratio of NUR to OUR rather reflects the rate of carbon source uptake (storage) under anoxic and aerobic conditions than growth process.

General information
State: Published
Organisations: Ghent University
Contributors: Sin, G., Malisse, K., Vanrolleghem, P.
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.34 SJR 0.429 SNIP 0.574
Web of Science (2017): Impact factor 1.247
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.404 SNIP 0.637
Web of Science (2016): Impact factor 1.197
Projects:

**ModLife: 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  
Sin, G., Project Coordinator, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Abildskov, J., Supervisor, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Zubov, A., Project Manager, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Al, R., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Ruszczyński, L., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
do Carmo Montes, F. D. C., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Ferro-Hernandez, H. A., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Jones, M. N., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
Project ID: 675251  
01/11/2015 → 31/10/2019  
Keywords: mathematical modeling, optimization, control, life sciences, biotechnology  
Collaborators: Imperial College London, Unilever, Universite Claude Bernard Lyon 1, Alfa Laval Copenhagen A/S, University of Strathclyde, Bayer, RWTH Aachen University  
Project: Research

**Sustainable Process Synthesis and Design**  
Al, R., PhD Student, Department of Chemical and Biochemical Engineering  
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering  
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering  
Zubov, A., Supervisor, Department of Chemical and Biochemical Engineering  
Marie Curie (EU-stipendium)  
01/05/2017 → 30/04/2020  
Award relations: Sustainable Process Synthesis and Design  
Project: PhD

**Advanced Modelling, Simulation and Optimization for in Silivo Process Design**  
Öner, M., PhD Student, Department of Chemical and Biochemical Engineering  
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering  
Abildskov, J., Supervisor, Department of Chemical and Biochemical Engineering  
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering  
Shibabaw Molla, G., Supervisor, Department of Chemical and Biochemical Engineering  
Stocks, S. M., Supervisor  
Freitag, M. F., Supervisor  
Samfinansieret - Andet  
01/01/2017 → 31/12/2019  
Award relations: Advanced Modelling, Simulation and Optimization for in Silivo Process Design  
Project: PhD

**Functional Modeling of water treatment system**  
Nielsen, E. K., PhD Student, Department of Electrical Engineering  
Ravn, O., Main Supervisor, Department of Electrical Engineering  
Lind, M., Supervisor, Department of Electrical Engineering  
Eksternt finansieret virksomhed  
01/10/2016 → 30/09/2019  
Award relations: Functional Modeling of water treatment system  
Project: PhD

**A Decision Support Tool for Screening Novel WWTP Processes**  
Behera, C. R., PhD Student, Department of Chemical and Biochemical Engineering  
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering  
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering  
Forskningsrådfinsaniering
A Decision Support Tool for Screening Novel WWT Processes

Behera, C. R., PhD Student
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Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering

Forskningsrådsfinansiering

15/08/2016 → 14/08/2019

Award relations: A Decision Support Tool for Screening Novel WWT Processes
Project: PhD

Thermodynamic modelling and data evaluation for life sciences applications

Ruszczynski, L., PhD Student, Department of Chemical and Biochemical Engineering
Abildskov, J., Main Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering
Zubov, A., Supervisor, Department of Chemical and Biochemical Engineering

Marie Curie (EU-stipendium)
01/05/2016 → 30/04/2019

Award relations: Thermodynamic modelling and data evaluation for life sciences applications
Project: PhD

Validation and Improvement of Property and Process Modelling for Oleochemicals

Forero-Hernandez, H. A., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Abildskov, J., Supervisor, Department of Chemical and Biochemical Engineering
Jensen, A. D., Supervisor, Department of Chemical and Biochemical Engineering
Sarup, B., Supervisor

Ansat eksternt
01/06/2016 → 31/05/2019

Award relations: Validation and Improvement of Property and Process Modelling for Oleochemicals
Project: PhD

In-silico Process Design and Evaluation Tool for Pharmaceutical Manufacturing

do Carmo Montes, F. D. C., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering

Marie Curie (EU-stipendium)
15/04/2016 → 14/04/2019

Award relations: In-silico Process Design and Evaluation Tool for Pharmaceutical Manufacturing
Project: PhD

Design and optimization of selected oleochemical processes

Jones, M. N., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Sarup, B., Supervisor

Ansat eksternt
15/04/2016 → 14/04/2019

Award relations: Design and optimization of selected oleochemical processes
Project: PhD

Bioprocess risk assessment using a mechanistic modelling framework

Spann, R., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Eliasson Lantz, A., Supervisor, Department of Chemical and Biochemical Engineering
Flores-Alsina, X., Examiner
Delvigne, F., Examiner
Stocks, S. M., Examiner
Alsina, X. F., Examiner
Stocks, S. M., Examiner
Marie Curie (EU-stipendium)
01/08/2015 → 31/07/2018
Award relations: Bioprocess risk assessment using a mechanistic modelling framework
Project: PhD

The implementation of anammox in a full-scale industrial waste-water treatment plant
Feldman, H., PhD Student, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Main Supervisor, Department of Chemical and Biochemical Engineering
Flores Alsina, X., Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering
Skiadas, I. V., Examiner, Department of Chemical and Biochemical Engineering
Vanrolleghem, P., Examiner, Department of Environmental Engineering
Volcke, E., Examiner
Volcke, E., Examiner
Samfinansierede - Virksomhed
01/04/2015 → 31/07/2018
Award relations: The implementation of anammox in a full-scale industrial waste-water treatment plant
Project: PhD

Computer-aided molecular design of novel working fluids to optimize heat transfer processes
Frutiger, J., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Abildskov, J., Supervisor, Department of Chemical and Biochemical Engineering
von Solms, N., Examiner, Department of Chemical and Biochemical Engineering
Bode, A., Examiner
Papadopoulos, A., Examiner
Bode, A., Examiner
Papadopoulos, A., Examiner
Forskningsrådssamfinansiering
01/06/2014 → 25/08/2017
Award relations: Computer-aided molecular design of novel working fluids to optimize heat transfer processes
Project: PhD

Exploring biochemical process performance limits through topology optimization
Larsson, H. K., PhD Student, Department of Chemical and Biochemical Engineering
Krühne, U., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Skov, A. L., Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Examiner, Department of Chemical and Biochemical Engineering
Drønen, N. K., Examiner
Nopens, I., Examiner
Grundforskningsfonden
01/12/2012 → 16/06/2016
Award relations: Exploring biochemical process performance limits through topology optimization
Project: PhD

Modelling and Optimization of Energy Systems for Off-Shore Platforms
Nguyen, T., PhD Student, Department of Mechanical Engineering
Elmegaard, B., Main Supervisor, Department of Mechanical Engineering
Haglind, F., Supervisor, Department of Mechanical Engineering
Sin, G., Examiner, Department of Chemical and Biochemical Engineering
Angelo, P., Examiner
de Oliveira Júnior, S., Examiner
Institut, samfinansiering
01/11/2011 → 26/01/2015
Award relations: Modelling and Optimization of Energy Systems for Off-Shore Platforms
Project: PhD

Performance Monitoring, Diagnosis and Advanced Control for Bio-Refinery
Prunescu, R. M., PhD Student, Department of Electrical Engineering
Optimizing control of the integrated urban wastewater system

Mollerup, A. L., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Mikkelsen, P. S., Supervisor
Gernaey, K. V., Examiner, Department of Chemical and Biochemical Engineering
Olsson, G., Examiner
Weijers, S. R., Examiner
ErhvervsPhD-ordningen VTU
01/08/2011 → 10/11/2015
Award relations: Optimizing control of the integrated urban wastewater system
Project: PhD

Control of Process Operations and Monitoring of Product Qualities through Hybrid Multi-Scale Model-Based Analysis

Abdul Samad, N. A. F. B., PhD Student, Department of Chemical and Biochemical Engineering
Gani, R., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering
Jørgensen, J. B., Examiner, Department of Chemical and Biochemical Engineering
Georgiadis, M. C., Examiner
Kalman Nagy, Z., Examiner
Stipendie fra udlandet
01/01/2009 → 21/11/2012
Award relations: Control of Process Operations and Monitoring of Product Qualities through Hybrid Multi-Scale Model-Based Analysis
Project: PhD

Integration of Modelling, Design and Control for Efficient Operation of Chemical Processes

Abd Hamid, M. K. B., PhD Student, Department of Chemical and Biochemical Engineering
Gani, R., Main Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Examiner, Department of Chemical and Biochemical Engineering
Manan, Z. A., Examiner
Skogestad, S., Examiner
Stipendie fra udlandet
01/07/2007 → 13/04/2011
Award relations: Integration of Modelling, Design and Control for Efficient Operation of Chemical Processes
Project: PhD

Multi-enzyme process modelling

Andrade Santacoloma, P. D. G., PhD Student, Department of Informatics and Mathematical Modeling
Woodley, J., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering
Jørgensen, S. B., Examiner, Department of Chemical and Biochemical Engineering
Pedersen, S., Examiner
Vasic-Racki, D., Examiner
Institut stipendie (DTU) Samf.
01/11/2008 → 27/06/2012
Award relations: Multi-enzyme process modelling
Project: PhD
Systematic Methods and Tools for Computer Aided Modeling
Fedorova, M., PhD Student, Novo Nordisk Foundation Center for Biosustainability
Gani, R., Main Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Examiner, Department of Chemical and Biochemical Engineering
Linninger, A. A., Examiner
Preisig, H. A., Examiner
Preisig, H. A., Examiner
Anden EU-finansiering
01/04/2012 → 02/09/2015
Award relations: Systematic Methods and Tools for Computer Aided Modeling
Project: PhD

Sustainable design of biorefinery systems for biorenewables
Loureiro da Costa Lira Gargalo, C., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Carvalho, A. I. C. D. S. G., Supervisor
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Flores Alsina, X., Examiner, Department of Chemical and Biochemical Engineering
Bezzo, F., Examiner
Matos, H. A. S. D., Examiner
Marie Curie (EU-stipendium)
15/11/2013 → 25/08/2017
Award relations: Sustainable design of biorefinery systems for biorenewables
Project: PhD

Tailor-made design of chemical products: Bio-fuels and other blended products
Yunus, N. A. B., PhD Student, Department of Chemical and Biochemical Engineering
Gani, R., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Woodley, J., Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Examiner, Department of Chemical and Biochemical Engineering
Harper, P. M., Examiner, Department of Chemical and Biochemical Engineering
Kate, A. J. B. T., Examiner
Stipendie fra udlændet
15/07/2010 → 07/05/2014
Award relations: Tailor-made design of chemical products: Bio-fuels and other blended products
Project: PhD

Integrated framework for synthesis and design of multi-product biorefinery networks
Cheali, P., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Huusom, J. K., Examiner, Department of Chemical and Biochemical Engineering
Mogensen, J., Examiner
Zondervan, E., Examiner
Institut stipendie (DTU) Samf.
01/05/2012 → 01/07/2015
Award relations: Integrated framework for synthesis and design of multi-product biorefinery networks
Project: PhD

Model Based Integrated Process-Product Design - retrofitting and optimisation
Hukkerikar, A. S., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Abildskov, J., Supervisor, Department of Chemical and Biochemical Engineering
Gani, R., Supervisor, Department of Chemical and Biochemical Engineering
Sarup, B., Supervisor
Kontogeorgis, G., Examiner, Department of Chemical and Biochemical Engineering
Frenkel, M., Examiner
Krooshof, G., Examiner
Ansat eksternt
01/07/2010 → 30/09/2013
Award relations: Model Based Integrated Process-Product Design - retrofitting and optimisation
Computer-aided modelling for efficient and innovative product-process engineering
Heitzig, M., PhD Student, Department of Chemical and Biochemical Engineering
Gani, R., Main Supervisor, Department of Chemical and Biochemical Engineering
Glarborg, P., Supervisor, Department of Chemical and Biochemical Engineering
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Examiner, Department of Chemical and Biochemical Engineering
Piccione, P. M., Examiner
Pistikopoulos, S. E., Examiner
Institut stipendie (DTU)
01/12/2008 → 18/04/2012
Award relations: Computer-aided modelling for efficient and innovative product-process engineering
Project: PhD

Validation of Structures Model for Autotrophic Nitrogen Removal in High Strength Wastewater
Vangsgaard, A. K., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Smets, B. F., Supervisor
Krühne, U., Examiner, Department of Chemical and Biochemical Engineering
Lemaire, R., Examiner
Morgenroth, E., Examiner
1/3 FUU, 1/3 inst 1/3 Andet
01/06/2010 → 12/11/2013
Award relations: Validation of Structures Model for Autotrophic Nitrogen Removal in High Strength Wastewater
Project: PhD

Plantwide modelling and control for N2O emissions fro WWTP
Boiocchi, R., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering
Abildskov, J., Examiner, Department of Chemical and Biochemical Engineering
Weijers, S. R., Examiner
Van Loosdrecht, M., Examiner
Samfinansieret - Andet
01/10/2013 → 14/12/2016
Award relations: Plantwide modelling and control for N2O emissions fro WWTP
Project: PhD

Incremental refinement of process design
Quaglia, A., PhD Student, Department of Chemical and Biochemical Engineering
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering
Gani, R., Supervisor, Department of Chemical and Biochemical Engineering
Sarup, B., Supervisor
Jørgensen, J. B., Examiner, Department of Chemical and Biochemical Engineering
Bode, A., Examiner
Pistikopoulos, E. N., Examiner
Marie Curie (EU-stipendium)
01/06/2010 → 30/09/2013
Award relations: Incremental refinement of process design
Project: PhD

Sustainable assessment of full chain bioenergy production
Saez de Bikuna Salinas, K., PhD Student, Department of Environmental Engineering
Ibrom, A., Main Supervisor, Department of Environmental Engineering
Hauschild, M. Z., Supervisor
Pilegaard, K., Supervisor, Department of Environmental Engineering
Damgaard, A., Examiner, Department of Environmental Engineering
Sin, G., Examiner, Department of Environmental Engineering
Damgaard, A., Examiner, Department of Environmental Engineering
Brandão, M. M. R., Examiner
**Computer aided framework for synthesis, design and retrofit of water networks in processing industries**

Bozkurt, H., PhD Student, Department of Chemical and Biochemical Engineering  
Sin, G., Main Supervisor, Department of Chemical and Biochemical Engineering  
Gernaey, K. V., Supervisor, Department of Chemical and Biochemical Engineering  
Krühne, U., Examiner, Department of Chemical and Biochemical Engineering  
Comas, J., Examiner  
Weijers, S. R., Examiner  
1/3 FUU, 1/3 inst 1/3 Andet  
16/12/2011 → 13/05/2015  
Award relations: Computer aided framework for synthesis, design and retrofit of water networks in processing industries  
Project: PhD

**Establishment and calibration of consensus process models of N2O dynamics**

Domingo-Felez, C., PhD Student, Department of Environmental Engineering  
Smets, B. F., Main Supervisor, Department of Environmental Engineering  
Plösz, B. G., Supervisor, Department of Environmental Engineering  
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering  
Gernaey, K. V., Examiner, Department of Chemical and Biochemical Engineering  
Plaza, E., Examiner  
Sperandio, M., Examiner  
Plaza, E., Examiner  
Sperandio, M., Examiner  
Samfinansieret - Andet  
15/12/2013 → 30/08/2017  
Award relations: Establishment and calibration of consensus process models of N2O dynamics  
Project: PhD

**Molecular and Microbial Analysis of Nitritation/Anammox Aggregates towards Optimization of Autotrophic Nitrogen Removal in Membrane Bioreactors**

Mutlu, A. G., PhD Student, Department of Environmental Engineering  
Smets, B. F., Main Supervisor, Department of Environmental Engineering  
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering  
Plösz, B. G., Examiner, Department of Environmental Engineering  
Joss, A., Examiner  
Wilén, B., Examiner  
Institut stipendie (DTU) Samf.  
01/01/2011 → 27/05/2015  
Award relations: Molecular and Microbial Analysis of Nitritation/Anammox Aggregates towards Optimization of Autotrophic Nitrogen Removal in Membrane Bioreactors  
Project: PhD

**Novel Strategies for Fermentation Control**

Mears, L., PhD Student, Department of Chemical and Biochemical Engineering  
Gernaey, K. V., Main Supervisor, Department of Chemical and Biochemical Engineering  
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering  
Sin, G., Supervisor, Department of Chemical and Biochemical Engineering  
Stocks, S. M., Supervisor  
Huusom, J. K., Examiner, Department of Chemical and Biochemical Engineering  
Glassey, J., Examiner  
Kold, D., Examiner  
Samfinansierede - Virksomhed  
01/12/2013 → 15/03/2017  
Award relations: Novel Strategies for Fermentation Control  
Project: PhD
**Modelling and Simulation of Wastewater Treatment Plants**
Snip, L., PhD Student, Department of Chemical and Biochemical Engineering
Gernaey, K. V., Main Supervisor, Department of Chemical and Biochemical Engineering
Flores-Alsina, X., Supervisor
Jeppsson, U. A. C., Supervisor
Krühne, U., Supervisor, Department of Chemical and Biochemical Engineering
Pilósz, B. G., Supervisor
Sin, G., Examiner, Department of Chemical and Biochemical Engineering
Ott, C., Examiner
Pons, M., Examiner
Marie Curie (EU-stipendium)
01/05/2012 → 01/07/2015
Award relations: Modelling and Simulation of Wastewater Treatment Plants
Project: PhD

**Computer Modelling of Lipid Processing Technology**
Diaz Tovar, C. A., PhD Student, Department of Chemical and Biochemical Engineering
Gani, R., Main Supervisor, Department of Chemical and Biochemical Engineering
Sarup, B., Supervisor
Sin, G., Examiner, Department of Chemical and Biochemical Engineering
Balchen, S., Examiner
Wiebe, L., Examiner
1/3 DTU-stip, 2/3 FUR/andet
01/05/2008 → 29/11/2011
Award relations: Computer Modelling of Lipid Processing Technology
Project: PhD

**THERMCYC: 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 surpass 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.
Elmegaard, B., Project Manager, Department of Mechanical Engineering, Thermal Energy
Haglind, F., Project Participant, Department of Mechanical Engineering, Thermal Energy
Claussen, L. R., Project Participant, Department of Mechanical Engineering, Thermal Energy
Kaern, M. R., Project Participant, Department of Mechanical Engineering, Thermal Energy
Markussen, W. B., Project Participant, Department of Mechanical Engineering, Thermal Energy
Sin, G., Project Participant, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Gani, R., Project Participant, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Meroni, A., PhD Student, Department of Mechanical Engineering, Thermal Energy
Andreasen, J. G., PhD Student, Department of Mechanical Engineering, Thermal Energy
Cignitti, S., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Frutiger, J., PhD Student, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Babi, D. K., Project Participant, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Serensen, I., Project Coordinator, Department of Mechanical Engineering
Pierobon, L., Project Participant, Department of Mechanical Engineering, Thermal Energy
Zhang, L., Project Participant, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Zühlsdorf, B., Project Participant, Department of Mechanical Engineering, Thermal Energy
Mancini, R., Project Participant, Department of Mechanical Engineering, Thermal Energy
Project ID: 76567
External Project ID: 1305-00036B
01/03/2014 → 28/02/2019
Collaborators: Maersk Group, Technical University of Munich, Danfoss AS, Arla Foods, Alfa Laval, MAN Diesel and Turbo, Viegand Maagae A/S, Delft University of Technology, Alfa Laval Copenhagen A/S, Aalborg University, Danish Technological Institute
Project: Research
Integrated modelling for simulation and design of novel enzymatic processes
An increasing number of industrially relevant enzymatic processes, including the production of biofuels, prebiotics and new chemicals by “green chemistry”, use solid or very viscous plant material as the raw material. These processes all depend on the parallel and/or serial action of multiple enzyme activities to produce the end products. Currently, the development and transfer of these processes from the proof-of-concept bench-scale stage to industrial scale are mainly done empirically and based on experiences from conventional one-pot conversion processes. This approach is rather inefficient and costly in terms of time and resource investments and may not even offer the most optimal and sustainable solutions. To resolve these challenges, this project aims to introduce a more rational model-based simulation framework for enzyme process design.

Sin, G., Project Manager, Department of Chemical and Biochemical Engineering
Project ID: 50551
Forskningsprojekter - Andre ministerier og styrelser: DKK1,886,400.00
01/02/2008 → 31/07/2010
Award relations: Integrated modelling for simulation and design of novel enzymatic processes
Project: Research

Activities:

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
In-Silico Tailoring Properties of Polylactide
Period: 13 Nov 2016 → 18 Nov 2016
Alexandr Zubov (Speaker)
Gürkan Sin (Other)
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Degree of recognition: International
Links:
https://aiche.confex.com/aiche/2016/webprogram/Paper470226.html

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

A Tool to Support Optimal Industrial Wastewater Treatment Design and Analysis
Period: 24 Apr 2013 → 26 Apr 2013
Gürkan Sin (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering

Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Design of future municipal wastewater treatment plants: A mathematical approach to manage complexity and identify optimal solutions
Period: 24 Apr 2013 → 26 Apr 2013
Gürkan Sin (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Department of Environmental Engineering

Description

Related event
Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Activity: Talks and presentations › Conference presentations

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

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

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations
Biorefinery Òresund 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 Òresund Conference 'Biorefining from raw material to high value products'
18/09/2013 → …
Ørestad, Denmark
Activity: Talks and presentations › Conference presentations

Press clippings:

Modeling for production of bacterial cultures
Gürkan Sin & Krist V. Gernaey
02/11/2018
Department of Chemical and Biochemical Engineering, Centre for oil and gas – DTU, KT Consortium, PROSYS - Process and Systems Engineering Centre

Media contribution (1)

Computermodel skyder genvej til produktion af nye bakterier
02/11/2018
Ingeniøren
Per Henrik Hansen
1 page
This is a summary highlight from the PhD project of Robert Spann at DTU Chemical Engineering about mechanistic modeling for risk based monitoring of LAB cultures. The work is supervised by assoc.prof. Gürkan Sin & Prof. Krist Gernaey both from DTU Chemical Engineering and in collaboration with Chr Hansen.
Gürkan Sin & Krist V. Gernaey
Department of Chemical and Biochemical Engineering, KT Consortium, PROSYS - Process and Systems Engineering Centre, Centre for oil and gas – DTU
Press/Media: Press / Media