**Rafiqul Gani - DTU Orbit (04/12/2017)**

**Rafiqul Gani**

**Organisations**

**Computer Aided Process Engineering Center**  
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**Publications:**

**Estimation of Physical Properties of Amino Acids by Group-Contribution Method**

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

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

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

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

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

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

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Authors: Papadakis, E. (Intern), Anantpinijwatna, A. (Ekstern), Woodley, J. (Intern), Gani, R. (Intern)
Chapter 3 – VPPD-Lab: The Chemical Product Simulator

Computer-aided methods and tools for current and future product–process design and development need to manage problems requiring efficient handling of models, data, and knowledge from different sources and at different times and size scales. In this chapter, a systematic model-based framework for computer-aided chemical product design and evaluation, implemented in the software called VPPD-Lab, is presented. In the same way a typical process simulator works, the VPPD-Lab allows users to: (1) analyze chemical-based products by performing virtual experiments (product property and performance calculations), (2) predict the properties of products, and (3) create new product property and product performance models when needed. However, unlike process simulators, VPPD-Lab can also be used directly for (1) design of chemicals based products using design templates for various types of products, such as single molecule products, formulations, blends, emulsions, and devices; and (2) to create new product design templates when the needed template for a desired product is not available. VPPD-Lab employs a suite of algorithms (such as database search, molecular and mixture blend design) and toolboxes (such as property calculations and property model consistency tests) for specific product property prediction, design, and/or analysis tasks. The application of VPPD-Lab is highlighted through case studies involving solvent mixture stability check, lubricant blend design, jet fuel blend design, and insect repellent lotion design. Through these case studies, the use of design templates, associated workflows (methods), data flows (software integration), and solution strategies (database and tools) are highlighted.
Chapter 6 – Computer-Aided Molecular Design and Property Prediction

Today’s society needs many chemical-based products for its survival, nutrition, health, transportation, agriculture, and the functioning of processes. Chemical-based products have to be designed/developed in order to meet these needs, while at the same time, they must be innovative and sustainable to meet the global challenges of resources, competition, and demand. Design/development of these products mostly follows experiment-based trial and error approaches. With the availability of reliable property prediction models, however, computer-aided techniques have become popular, at least for the initial stages of the design/development process. Therefore, computer-aided molecular design and property prediction techniques are two topics that play important roles in chemical product design, analysis, and application. In this chapter, an overview of the concepts, methods, and tools related to these two topics are given. In addition, a generic computer-aided framework for the design of molecules, mixtures, and blends is presented. The application of the framework is highlighted for molecular products through two case studies involving the design of refrigerants and surfactants.

Designing a Surrogate Fuel for Gas-to-Liquid Derived Diesel

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

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Energy efficiency as an example of cross-discipline collaboration in chemical engineering

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

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

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

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

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

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Property Model-Based Chemical Substitution and Chemical Formulation Design

Chemical-based products including structured product formulations and single molecule products have proven to be a boon to mankind and have been a significant part of our economies. Our life and the changes around us cannot be imagined without the presence or involvement of chemicals. But like every coin has two sides, some chemicals constituting these products can also be a curse. This is primarily due to the hazardous environment-related properties that some of these chemicals possess and there are many more chemicals which have not been evaluated due to lack of resources for rigorous, experimental-based estimation methods [1]. Hence, there is a dire necessity to identify such chemicals which may be dangerous to the environment, toxic to human health and harmful for our fragile eco-system. Besides, in many cases, their corresponding chemical production processes generate harmful emissions, which also have severe impacts on the environment. The concern about the environment and human health has given rise to the REACH regulation implemented by the European Chemical Agency (ECHA), which compels European chemical companies to stop the use of hazardous substances and replace them with environmentally benign chemicals. Additionally, the decisions taken during chemical product design also have an impact on the process and product performance and are influenced by company strategy, availability of market and government policies [2]. Hence, undoubtedly there is a need to develop a systematic, model-based methodology that can help to find substitutes to existing chemicals in order to improve process economics, operability as well as the sustainability, while still delivering the same or improved product functionality. It is useful to start with making structured databases by collecting data from knowledge base, followed by the development of predictive group-contribution property models and then the development of a general methodology for the model-based chemical substitution and chemical product design. The objective here is to quickly and reliably identify the promising candidates through model-based techniques and then to verify and evaluate their performance and applicability through experiments. In this way, the experimental resources are used for verification rather than for an inefficient, trial-and-error search used for practically all chemical products. Besides, when it is desired to come up with alternative substitutes for the undesirable chemicals, the trial an error based approach will have a very large search space. This could be avoided by having predictive models coupled with the desired target properties, making the identification of these substitutes easier. The goal therefore is to investigate comprehensively the uses and properties of the chemicals of concern; develop a systematic framework to identify, compare and select safer alternatives to these including their corresponding manufacturing processes; and finally design safe chemical product formulations or product formulations with improved product performance. The model-based approach makes use of validated property models to identify the chemicals which need to be substituted, that is, the chemicals that meet the desired physico-chemical properties but not the regulatory (EH&S: environmental, health and safety) properties, and then to generate, evaluate and identify candidates that can replace them. The presentation will discuss the general methodology for chemical substitution, which caters to different problem definitions depending on the reason for substitution. The associated property modeling tools [3] will also be highlighted. A set of new group contribution-based models for a number of useful properties of amino acids will be presented. Through examples on substitution of chemicals from chemical-based products from various sectors namely cosmetics and personal care, pharmaceutical and food, with amino acids (as active ingredient or as additive) will be shown along with other well-known substitution problems. These examples will also highlight the role of property models in chemical substitution and chemical product formulation.

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A Generic Methodology for Superstructure Optimization of Different Processing Networks

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

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A Generic Methodology for Superstructure Optimization of Different Processing Networks

A large focus is placed on sustainability and sustainable practices as a result of the arising environmental issues. As an element of this, sustainable process synthesis and design becomes important. A generic, systematic methodology is proposed for solving the problem of optimal design of sustainable processing networks containing three stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. In this work, a focus is placed on the first stage, the synthesis stage. Process synthesis becomes necessary in determining the appropriate processing routes to produce a selection of products from a set or feedstock. The problem to be solved here is the following: for a given set of raw materials, products and a network of processing routes, determine the optimal processing route from a sustainability point of view. Three different processing networks arising from chemical processes, biorefineries, and carbon dioxide utilization are considered. In the synthesis stage, the processing alternatives are represented in a superstructure and the associated data is collected and stored in a database. Once a specific process synthesis problem is formulated, the existing superstructure is retrieved and reduced in order to include only the relevant alternatives. New alternatives can easily be added and stored in the database. The superstructure of alternatives in the network is then represented using a generic data-independent process model, which yields a mixed integer linear or nonlinear programming problem. The proposed methodology involves the use of additional methods and tools, such as a database and an external software for solving the network
optimization problem. The database has been created using an ontology-based knowledge representation consisting in various layers of data and interconnections between them. Using a common database structure for any process synthesis problem allows for easy data collection, storage and retrieval, as well as giving the possibility of solving combined problems that have been previously solved independently. The step-by-step methodology has been implemented in a software interface that guides the user through the problem formulation and solution steps and integrates the various methods and tools for efficient flow of information between them. By using this interface, the user can retrieve and/or modify existing networks and alternatives from the database, as well as add new alternatives and connections between them. With the generated superstructure of alternatives and the corresponding data, an input file for GAMS is automatically created. This input file contains values of all the parameters of the generic process model. Then, the problem is solved in GAMS and the interface shows the results and allows for the selection of alternatives. The output from the synthesis stage (the first stage) is the optimal processing route for the defined problem and scenario, which can be transferred to a rigorous process simulator for the second stage (design stage). Here, the selected route needs to be further designed, simulated and analyzed. Then, more sustainable innovative designs can be developed in the third stage based on the output design from the second stage. This generic methodology and software interface can be applied to an array of problems within synthesis of processing networks. This is illustrated through case studies from two applications: the synthesis of biorefinery networks and the synthesis of sustainable carbon dioxide utilization processes.

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**Organisations:** Department of Chemical and Biochemical Engineering, CAPEC-PROCESS  
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**A generic methodology for the design of sustainable carbon dioxide utilization processes using superstructure optimization**

Global warming and other environmental concerns are fueling increased focus on sustainability resulting in new and stringent guidelines, especially with regard to emissions [1]. Greenhouse gases are prevalent and among harmful emissions that are targeted to be reduced; carbon dioxide (CO2) is the primary greenhouse gas that is targeted via carbon capture and storage (CCS) as well as carbon capture and utilization (CCU) [1]. Carbon capture and utilization is showing promise because, in contrast with carbon capture and storage, it takes the captured carbon dioxide and makes further use of it, including as an extractive agent or raw material. Chemical conversion, an important element of utilization, involves the use of carbon dioxide as a reactant in the production of chemical compounds [2]. However, for feasible implementation, a systematic methodology is needed for the design of the utilization, especially chemical conversion, processes. To achieve this, a generic methodology has been developed, which adopts a three-stage approach consisting in (i) process synthesis, (ii) process design, and (iii) innovative and sustainable design [3]. This methodology, with the individual steps and associated methods and tools, has been developed and applied to carbon dioxide utilization networks.

This work will focus on the first stage, process synthesis, of this three-stage methodology; process synthesis is important in determining the appropriate processing route to produce products from a selection of feedstock [4], in this case carbon dioxide. This stage contains three steps, each incorporating relevant methods and tools. First, with the help of user specifications, the problem is specified. Then, the processing routes linking feed and product are represented via a superstructure. This is performed with the help of a software interface, Super-O, guiding through the steps of the methodology related to superstructure development and optimization [5]. The data necessary to perform this step is extracted from an especially structured database ontologically designed for the easy extraction and addition of data. This database contains information on the raw material (including different carbon dioxide emission conditions), the products and the reactions linking these. With this help of the database it is possible to quickly compare utilization processes for a specific problem as the information is easily accessible; thereby, for the problem of certain products and given a specific feed it becomes easy to say which conversion processes are most promising to sustainably reduce emissions.

This methodology, the software interface and the database will be presented together with validation results from a conceptual example. Using the methodology a network of conversion reactions from carbon dioxide to various carbon, hydrogen and oxygen containing compounds, such as methanol, dimethyl ether and dimethyl carbonate, is developed; using ProCARP [6], a software tool for reaction path synthesis, the network is created containing the feasible reactions. Using the developed database, the data needed, including reaction conversions and separation factors, for the superstructure is extracted. The optimization gives the selection of the best processing routes. These are subsequently designed rigorously and analyzed for economic and environmental sustainability. The resulting design and analysis show the use of the methodology and the opportunity for sustainable reduction of emissions using conversion processes to produce chemical products.
A grand model for chemical product design

Chemical engineering has been expanding its focus from primarily business-to-business products (B2B) to business-to-consumer (B2C) products. The production of B2B products generally emphasizes on process design and optimization, whereas the production of B2C products focuses on product quality, ingredients and structure. Market and competitive analysis, government policies and regulations have to be explicitly considered in product design. All these considerations are accounted for in the Grand Product Design Model, which consists of a process model, a property model, a quality model, a cost model, a pricing model, an economic model as well as factors such as company strategy, government policies and regulations. This article introduces the model and highlights selected aspects of the model with two case studies. One is a die attach adhesive that illustrates how pricing affects profitability, and how product composition changes with market conditions. Another is a hand lotion that illustrates how product quality affects the profit. (C) 2016 Elsevier Ltd. All rights reserved.
A methodological framework for the development of feasible CO₂ conversion processes
Converting captured CO₂ feedstock into valuable chemical products is viewed as one of the potential ways to reduce atmospheric CO₂ emission. To this end, a methodological framework is suggested to support the development of feasible CO₂ conversion processes that can contribute to the CO₂ reduction by replacing non-CO₂ utilizing processes or non CO₂ -based products. The framework encompasses several execution and decision steps and uses three main criteria, which are the demand availability, CO₂ reduction feasibility, and economic feasibility. As an illustrative example, a methanol plant employing combined reforming (CR) of methane reaction is developed. To supply the CO₂ feedstock, the aMDEA-based CO₂ capture applied to a SMR-based H₂ plant is considered. A baseline process is developed and is compared with a non-CO₂ utilizing conventional methanol plant (process substitution) and a gasoline production process (product substitution) in terms of the established criteria. For the former, it is verified that the methanol production via combined reforming leads to cheaper unit production cost as well as lower net CO₂ emission compared to the conventional methanol plant. For the latter, it is shown that the feasibility of the CO₂-based methanol as an alternative fuel to gasoline highly depends on the type and price of the raw materials. To improve the developed baseline CO₂ conversion process further, (1) some of the combined reforming reaction related design variables are fine-tuned using a sensitivity analysis and an equilibrated syngas plot, and (2) utilization of various renewable energy resources for the internal electricity demand is examined.

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A methodology for the sustainable design and implementation strategy of CO₂ utilization processes

This work presents a systematic methodology that has been developed for the design of sustainable CO₂ utilization processes that can mitigate CO₂ and also guarantee profitability. First, the three-stage methodology, evaluation criteria and applicable tools are described. Especially, the process design and analysis is discussed as only limited amounts of process data is available for determining the optimal processing path and in the third stage the issue of implementation strategy is considered. As examples, two CO₂ utilization methods for methanol production, combined reforming and direct synthesis are considered. Methanol plants employing such methods are developed using synthesis-design and simulation tools and their evaluation indicators are calculated under various implementation strategies. It is demonstrated that integrating or replacing an existing conventional methanol plant by a combined reforming method represents a sustainable solution. Additionally, producing methanol through direct hydrogenation is a promising way to convert CO₂ when cheap H₂ feeds are available.

General information

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Analysis and modeling of alkali halide aqueous solutions

A new model is proposed for correlation and prediction of thermodynamic properties of electrolyte solutions. In the proposed model, terms of a second virial coefficient-type and of a KT-UNIFAC model are used to account for a contribution of binary interactions between ion and ion, and water and ion, respectively, with a Debye-Hückel term for electrostatic interactions. In a second approach of the model, additional parameters for interactions of ion pairs in the KT-UNIFAC are introduced as a correction to get better agreement with data. Structural parameters of ions used in the framework of UNIFAC or UNIQUAC are newly estimated using ionic radii for physically correct representation of the combinatorial part. Including temperature-dependent coefficients in the interaction parameters, significant improvements in accuracy are achieved for a wide range of temperatures. This work is focused on calculations for various electrolyte properties of alkali halide aqueous solutions such as mean ionic activity coefficients, osmotic coefficients, and salt solubilities. The model covers highly nonideal electrolyte systems such as lithium chloride, lithium bromide and lithium iodide, that is, systems that are very soluble in water, for example, up to more than 30 mol kg⁻¹. Phase behaviors for the systems are analyzed at concentrations of salt up to the solubility in water at temperatures between 273 and 373 K by comparing calculated results with available experimental data and available models.

General information

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As concerns about the environment are growing, new efforts are needed to achieve more sustainable processes. One such environmental concern is global warming, which is primarily caused by the greenhouse effect or the increase in concentration of greenhouse gases [1]. The most significant greenhouse gases are carbon dioxide, methane and nitrous oxide, of which carbon dioxide is the highest constituent at 82%. Furthermore, the amount of carbon dioxide emissions is growing with time. These trends make it evident that there is a need for methods to reduce these greenhouse gases emissions. While there are two methods of reducing carbon dioxide emissions, carbon capture and storage (CCS) and carbon capture and utilization (CCU), CCU is considered promising as it makes further use of the carbon dioxide as a solvent, raw material, and reagent to produce valuable products [1]. Using such utilization processes, the emissions can be reduced as they are being utilized and profit can be obtained, or the cost of operation for the carbon dioxide treatment can be returned, through this utilization process.

In order to systematically reduce such emissions, carbon capture and utilization is considered rather than carbon capture and storage. To achieve this a methodology is developed to design sustainable carbon dioxide utilization processes. First, the information on the possible utilization alternatives is collected, including the economic potential of the process and the carbon dioxide emissions. The carbon dioxide emissions can be classified as direct and indirect emissions in a chemical process. The net carbon dioxide is determined for the utilization processes as the indirect carbon dioxide emissions minus the carbon dioxide utilized. Processes that presents zero or negative net carbon dioxide emission are desired in order to reduce the carbon dioxide emissions. Using this estimated preliminary evaluation, the top processes, with the most negative carbon dioxide emission are investigated by rigorous detailed simulation to evaluate the net carbon dioxide emissions. Once the base case design is established and evaluated, targeted improvements are made by exploiting opportunities, for example, optimization, heat integration and improved design decisions so that more sustainable and
lower net carbon dioxide emission alternatives are obtained. This method is applied to various processes where carbon dioxide is used as raw material. First, the process data are collected and compared. The economic feasibility is evaluated. From this, five processes are selected and analyzed in detail: the production of dimethyl carbonate, succinic acid, propylene carbonate, dimethyl ethylene and methanol. Not all the studied processes could be designed for zero or negative net carbon dioxide emission. Propylene carbonate production is found to have a negative net carbon dioxide, where, implementing targeted process improvements minimized the net carbon dioxide emission to -0.389 kg of carbon dioxide per kg of propylene carbonate. On the other hand, for succinic acid production, even after targeted improvements, the net carbon dioxide remained positive, even though compared to the existing industrial processes there is a relative reduction of up to 85%.

What this study shows is that for meaningful net carbon dioxide reduction, the carbon dioxide utilization processes need to be selected very carefully to obtain the best results. However, the opportunity to potentially reduce the net carbon dioxide emissions for the production of some bulk chemicals with carbon dioxide as feedstock exists.
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A Systematic Modelling Framework for Phase Transfer Catalyst Systems

Phase-transfer catalyst systems contain two liquid phases, with a catalyst (PTC) that transfers between the phases, driving product formation in one phase and being regenerated in the other phase. Typically the reaction involves neutral species in an organic phase and regeneration involves ions in an aqueous phase. These reacting systems are receiving increased attention as novel organic synthesis options due to their flexible operation, higher product yields, and ability to avoid hazardous or expensive solvents. Major considerations in the design and analysis of PTC systems are physical and chemical equilibria, as well as kinetic mechanisms and rates. This paper presents a modelling framework for design and analysis of PTC systems that requires a minimum amount of experimental data to develop and employ the necessary thermodynamic and reaction models and embeds them into a reactor model for simulation. The application of the framework is made to two cases in order to highlight the performance and issues of activity coefficient models for predicting design and operation and the effects when different organic solvents are employed.

General information

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Computer-Aided Sustainable Process Synthesis-Design and Analysis

Process synthesis involves the investigation of chemical reactions needed to produce the desired product, selection of the separation techniques needed for downstream processing, as well as taking decisions on sequencing the involved separation operations. For an effective, efficient and flexible design approach, what is needed is a systematic way to identify the types of tasks-operations that need to be performed, the corresponding design of the operation-equipment, their configuration, mass-energy flows, etc., giving an optimal flowsheet. Due to the fact that process synthesis problems are by nature combinatorial and open ended, a number of different solution approaches have been proposed. However the solution for any synthesis-design problem is dependent on the search space of alternatives and the process performance criteria which in most cases are influenced by economic factors. This work focuses on the development and application of a computer-aided framework for sustainable synthesis-design and analysis of process flowsheets by generating feasible alternatives covering the entire search space and includes analysis tools for sustainability, LCA and economics. The synthesis method is based on group contribution and a hybrid approach, where chemical process flowsheets are synthesized in the same way as atoms or groups of atoms are synthesized to form molecules in computer aided molecular design (CAMD) techniques. The building blocks in flowsheet synthesis problem are called as process-groups, which represent a single or set of unit operations that are selected by employing a thermodynamic insights based method. These building blocks are then combined using connectivity rules to generate all the feasible flowsheet alternatives. The main advantage of representing the flowsheet with process-groups is that, the performance of the entire process can be evaluated from the contributions of the individual process-groups towards the selected flowsheet property (for example, energy consumed). The developed flowsheet property models include energy consumption, carbon footprint, product recovery, product purity etc. In this way, the entire list of feasible chemical process flowsheets are quickly generated, screened and selected for further analysis. In the next stage, the design of the most promising process flowsheet candidates is performed through a reverse simulation approach, where the design parameters of the unit operations in the process flowsheet are calculated from selected process-groups definition. In the next stage the selected design is analyzed, for identifying process limitations or bottlenecks (hot-spots) using a comprehensive analysis method consisting of economic, life cycle and sustainability factors that are translated into design targets. In the final stage the identified hot-spots are targeted for overall process improvement and to generate innovative designs.
In this work the developed framework along with the associated methods and tools is tested through three case studies related to both chemical and biochemical industry in order to ascertain the applicability of the framework. In each of the cases numerous alternatives of novel and designs reported by others are quickly generated and evaluated. In all the case studies tested, the final design generated by the framework was novel and more sustainable.

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Development of a Model for a Continuous Ultra-Filtration System
Due to the wide applicability and simplicity of the ultra-filtration process, it is currently being used in a variety of commercial processes for the purpose of separation and concentration of valuable products and/or recovery of raw materials from dilute systems [1]. A predictive model for a system derived from first principles, is instrumental in evading the costs of conducting time-consuming experiments while also allowing one to not be dependent on a trial and error analysis approach. The validated final model can serve to understand the operational issues of the process and from it identify the important phenomena occurring in the process and/or the corresponding model parameters. Also, it can help to design experiments to collect useful measured data.

Therefore, a model was systematically developed in four phases: define the system to be modelled; derive the model equations representing the system; analyze and numerically solve the model equations; calibrate, validate and apply the model for different studies [2]. The objectives for the model are that it should be able to predict the feed and retentate flow-rates along with the permeate flux from a continuous ultra-filtration (UF) system consisting of different geometry (and ‘N’ membrane stacks) used for the concentration of enzyme solutions from a known inlet concentration to a desired (target) outlet concentration during the recovery and/or downstream processing of enzymes. The envisaged purpose of this model is to improve the efficiency of the UF separation process. The final model, saved as a model object, should be possible to use for the specified objectives as well as model parameter sensitivity, importance of the involved phenomena (mass transfer, permeability, etc.). Also, the model object could be used in an external simulation environment to guide process operators to run the system under different operational scenarios, such as operate at flow-rates specifically needed to take specified feed solutions to the desired outlet concentrations; or, to optimise the feed concentration to complete the process in a fixed time and many more. This could reduce the energy requirements when compared to running the process at the maximum pump flow-rate.

The developed steady-state model equations are organized in terms of conservation equations, constitutive equations and connection equations. Changing the process geometry changes the conservation and connection equations. Changing the model assumptions and/or the chemical system or involved phenomena, changes the constitutive equations. Therefore, from a master generic model, different versions of problem specific models are generated and used for different model scenarios. For example, different candidate models for filtration through UF membranes, which could describe the possible phenomenon occurring during the UF process (for example concentration polarization, pore blocking, cake formation, adsorption on the membrane) [3] have been generated and their performance compared and evaluated by using different sets of constitutive equations in the model. The connection equations were formulated to relate the retentate and permeate concentrations by the retentivity of the membrane.

Among the different models studied, the performance of a modified gel polarisation model was identified and was found to yield good results. Experimental data from the literature was used to estimate the parameters of the model, i.e., the mass transfer coefficients and an operational parameter, the gelling concentration, could be estimated for each enzyme using a least-squares fit of the objective function. The mass transfer coefficient from theoretical relations is known to be a function of the feed concentration or the gelling concentration of the enzyme, depending on the operational scenario. This result also confirmed observations reported in published papers on this subject [5]. Considering that, the velocity of flow and the membrane spacer dimensions are almost constant throughout the system, the mass transfer coefficient was found to vary only with the feed concentration. Lastly, the model was validated against experimental data and can predict the flow-rates within a difference of +/−20% of the experimental
The presentation will provide details of the developed model; the modelling tool used to develop, analyse and solve the model equations; estimation and sensitivity analysis of important model parameters; and the comparison and validation of the model behaviour with published data.

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**Early-Stage Design and Analysis of Biorefinery Networks**

The limited resources of fossil fuel as well as other important driving forces (e.g., environmental, social, and sustainability concerns) are expected to shape the future development of the chemical processing industries. These challenges motivate the development of new and sustainable technologies for the production of fuel, chemicals, and materials from renewable feedstock instead of fossil fuel. An emerging technology in response to these challenges is the biorefinery concept. The biorefinery is defined as the set of processes converting a bio-based feedstock into products such as fuels, chemicals, materials, and/or heat and power.

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**Authors:** Cheali, P. (Intern), Quaglia, A. (Intern), Loureiro da Costa Lira Gargalo, C. (Intern), Gernaey, K. (Intern), Sin, G. (Intern), Gani, R. (Intern)

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**Fundamentals of process intensification: A process systems engineering view**

This chapter gives an overview of the fundamentals of process intensification from a process systems engineering point of view. The concept of process intensification, including process integration, is explained together with the drivers for applying process intensification, which can be achieved at different scales of size, that is, the unit operation scale, the task scale, and the phenomena scale. The roles of process intensification with respect to process improvements and the generation of more sustainable process designs are discussed and questions related to when to apply process intensification and how to apply process intensification are answered through illustrative examples. The main issues and needs for generation of more sustainable process alternatives through process intensification are discussed in terms of the need for a systematic computer-aided framework and the methods and tools that should be employed through it. The process for the production of methyl-acetate is used as an example to highlight the generation of more sustainable process alternatives through this framework. Perspectives, conclusions, and future work are proposed in order to further develop the field of process intensification using a systems approach.

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Biphasic reaction systems are composed of immiscible aqueous and organic liquid phases where reactants, products, and catalysts are partitioned. These biphasic conditions point to novel synthesis paths, higher yields, and faster reactions, as well as facilitate product separation. The biphasic systems have a broad range of application, such as the manufacture of petroleum-based chemicals, pharmaceuticals, and agro-bio products. Major considerations in the design and analysis of biphasic reaction systems are physical and chemical equilibria, kinetic mechanisms, and reaction rates.

The primary contribution of this thesis is the development of a systematic modelling framework for the biphasic reaction system. The developed framework consists of three modules describing phase equilibria, reactions and mass transfer, and material balances of such processes. Correlative and predictive thermodynamic models, including newly developed group-contribution electrolyte model (e-KT-UNIFAC), have been implemented to predict the partitioning and equilibria of electrolyte and non-electrolyte species for a wide variety of reacting substances. Reaction kinetics and mass transfer are described by non-elementary reaction rate laws. Extents of reaction are used to calculate the species material balances. The resulting mathematical model contains temperature dependent reaction rate parameters, equilibrium constants, and partition coefficients; where only the reaction rates are to be regressed to a minimum of time-dependent data. The application of the framework is made to five distinct cases in order to highlight the performance of the model for correlating the data and predicting the overall rates, the ultimate amounts of product formation, the ultimate impurities amount, and the optimum operating condition using different organic solvents leading to an improved and innovative design of the system.
create new product design templates when the desired template is not available. The product design templates follow the same common steps in the workflow for a product type but have options to employ product specific property models, data and calculation routines, if necessary. This paper highlights the application of the templates for three case studies: (i) the design of a refrigeration cycle, (ii) a mixture/blend design problem involving lubricant design and (iii) a tailor-made product design of jet-fuels (blended chemical products).

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Chemical product design, Blended product, Refrigeration cycle

**Integrated Process Design and Control of Multi-element Reactive Distillation Processes**
In this work, integrated process design and control of reactive distillation processes involving multi-elements is presented. The reactive distillation column is designed using methods and tools which are similar in concept to non-reactive distillation design methods, such as driving force approach. The methods employed in this work are based on equivalent element concept. This concept facilitates the representation of a multi-element reactive system as equivalent binary light and heavy key elements. First, the reactive distillation column is designed at the maximum driving force where through steady-state analysis it is shown that it has the least energy consumption and carbon footprint. Next, through analytical and dynamic analysis it is verified that the control structure, disturbance rejection and the controllability at the maximum driving force is the best compared to any other design alternative which does not operate at the maximum driving force.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidad Autonoma Metropolitana
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Reactive distillation, Process design, Process Control, Multi-element system, Driving force

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Integrated Process Design, Control and Analysis of Intensified Chemical Processes

Process design and process control have been considered as independent problems for many years. In this context, a sequential approach is used where the process is designed first, followed by the control design. However, this sequential approach has its limitations related to dynamic constraint violations, for example, infeasible operating points, process overdesign or under-performance. Therefore, by using this approach, a robust performance is not always guaranteed. Furthermore, process design decisions can influence process control and operation. To overcome these limitations, an alternative approach is to tackle process design and controllability issues simultaneously, in the early stages of process design. This simultaneous synthesis approach provides optimal/near optimal operation and more efficient control of conventional (non-reactive binary distillation columns) as well as complex chemical processes; for example, intensified processes such as reactive distillation. Most importantly, it identifies and eliminates potentially promising design alternatives that may have controllability problems later. To date, a number of methodologies have been proposed and applied on various problems to address the interactions between process design and control, and they range from optimization-based approaches to model-based methods.

In this work, integrated process design and control of reactive distillation processes is considered through a computer-aided framework. To assure that design decisions give the optimum operational and economic performance, operability and controllability issues are considered simultaneously with the process design issues. Operability issues are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at imposed disturbances in the feed under normal operating conditions. First, a set design methods, similar in concept to design of non-reactive distillations, such as McCabe-Thiele and driving force approach are selected to design the reactive distillation column. Next, these design methods are extended using element concept to also include ternary as well as multicomponent reactive distillation processes. The element concept is used to translate a ternary system of compounds (A + B ↔ C) to a binary system of elements (WA and WB). When only two elements are needed to represent the reacting system of more than two compounds, a binary element system is identified. In the case of multi-element reactive distillation processes (where more than two elements are encountered) the equivalent element concept is used to translate a ternary system of compounds (A + B ↔ C + D) to a binary system of key elements (elements W_hk and W_Lk). For an energy-efficient design, non-reactive driving force (for binary non-reactive distillation), reactive driving force (for binary element systems) and binary-equivalent driving force (for multicomponent reactive distillation) were employed. For both the McCabe-Thiele and driving force method, vapor-liquid equilibrium data are based on elements. It has been is demonstrated that designing a reactive distillation column at the maximum driving force will result in the minimum energy consumption. Note, that the same principles that apply to a binary non-reactive compound system are valid also for a binary-element or a multi-element system. Therefore, it is advantageous to employ the element based method for multicomponent reaction-separation systems.

It is shown that the same design-control principles that apply to a non-reacting binary system of compounds are also valid for a reactive binary system of elements or multi-elements for distillation columns. Application of this framework shows that designing the reactive distillation process at the maximum driving force results in a feasible and reliable design of the process as well as the controller structure. Through analytical, steady-state and closed-loop dynamic analysis it is verified that the control structure, disturbance rejection and energy requirement of the reactive distillation column is better than any other operation point that is not at the maximum driving force. Furthermore, it is shown that the design at the maximum driving force can be both controlled using simple controllers such as PI as well as advanced controllers such as MPC.
Ionic Liquid Design and Process Simulation for Decarbonization of Shale Gas

Ionic liquids (ILs) have been receiving increasing attention as a potential decarbonization solvent. However, the enormous number of potential ILs that can be synthesized makes it a challenging task to search for the best IL for CO₂ removal from methane. In this work, a method was proposed to screen suitable ILs based on the COSMO-RS (conductor-like screening model for real solvents) model, an absorption mechanism, and experimental data. Besides the Henry’s constant, the viscosity and toxicity of ILs should also be taken into consideration for an industrial decarbonization process. Furthermore, process simulation was performed to evaluate the new IL-based decarbonization technology. Considering CO₂ solubility, CO₂/CH₄ selectivity and toxicity and viscosity of ILs, [bmim][NTf₂] has been screened to be the potential solvent among 90 classes of ILs. Based on reliable experimental data, a rigorous thermodynamic model was established. The simulation results have been found to agree well with the available experimental results. Two process flow sheet options, use of two single-stage flash operations or a multistage flash operation following the absorber, have been simulated and assessed. Compared with the well-known MDEA (methylene-diethanolamine) process for CO₂ capture, the single-stage and multistage process alternatives would reduce the total energy consumption by 42.8% and 66.04%, respectively.

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Modelling and synthesis of pharmaceutical processes: moving from batch to continuous

Research in pharmaceutical process development has gained a lot of interest over the last years. Long development times, increasing R&D costs, increasing competition, and short patent duration are some of the driving forces for the increased research efforts in the field. Increased process understanding of the pharmaceutical process has resulted in major improvements in the field. Process systems engineering (PSE) approaches, which have been successfully applied in the design, analysis and optimization of chemical and petrochemical processes, might be also important for the improvement of pharmaceutical processes by providing systematic and structured solutions for the stages of the pharmaceutical process development.

In this PhD thesis, the objective is to systematize the pharmaceutical process development in order to enhance process understanding by creating a data-rich environment and to investigate/evaluate opportunities for continuous operation. To achieve the mentioned objectives the use of an integrated framework based on systematic model-based methods and tools is proposed. Computer-aided methods and tools are used to generate process knowledge and to evaluate different operational scenarios.

The developed framework is divided into four main sections: the reaction pathway, reaction analysis, separation synthesis and process evaluation-operation based on evaluation. In the first section, the selection of the reaction pathway to produce a desired active ingredient is examined. A reaction database for small pharmaceutical molecules, including information for reactions, the solvent role and processing information, has been developed to assist the reaction pathway selection. In the second section, the reaction analysis, the identified individual reactions during the reaction pathway selection are analysed. The objective of the reaction analysis section is to collect reaction data and by using model-based methods to investigate possibilities of reaction improvement by evaluating the reaction conditions, the operating mode, the solvent role, and the reactor design. In the third section, alternatives for the separation of the reaction mixture are generated based on the driving force principles and evaluated based on performance criteria, such as mass and energy utilization. Finally, the overall process is simulated and evaluated in terms of productivity and environmental impact.

Process optimization studies are performed by defining optimization target based on the process analysis. The application of the developed integrated framework is highlighted through four case studies. In the first case study, the overall use of the framework is highlighted using the synthesis of ibuprofen as a motivating example. The second case study focuses on the application of the developed solvent selection methodology for solvent swap problems. The third case study focused on multiphase reaction systems and improvements through the combination of reaction-separation. Finally, model-based analysis-design is performed for the operation improvement of a glucose isomerization plant.
Models and Modelling Tools for Chemical Product and Process Design

The design, development and reliability of a chemical product and the process to manufacture it, need to be consistent with the end-use characteristics of the desired product. One of the common ways to match the desired product-process characteristics is through trial and error based experiments, which can be expensive and time consuming. An alternative approach is the use of a systematic model-based framework according to an established work-flow in product-process design, replacing some of the time consuming and/or repetitive experimental steps. The advantages of the use of a model-based framework is that in the design, development and/or manufacturing of a chemical product-process, the knowledge of the applied phenomena together with the product-process design details can be provided with diverse degrees of abstractions and details. This would allow the experimental resources to be employed for validation and fine-tuning of the solutions from the model-based framework, thereby, removing the need for trial and error experimental steps. Also, questions related to economic feasibility, operability and sustainability, among others, can be considered in the early stages of design. However, are the needed models for such a framework available? Or, are modelling tools that can help to develop the needed models available? Can such a model-based framework provide the needed model-based workflows matching the requirements of the specific chemical product-process design problems? What types of models are needed for innovative and more sustainable design? The presentation will review the current state of the art in models and modelling tools suitable for chemical product-process design and point out the gaps that need to be filled out with respect to model-based frameworks for chemical product-process design. Illustrative examples highlighting the need for efficient model-based systems will be presented, where the need for predictive models for innovative chemical product-process design will be highlighted. The examples will cover aspects of chemical product-process design where the idea of the grand chemical product design model, that also incorporates the process design issues together with sustainability issues will be presented.

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**New Vistas in Chemical Product and Process Design**

Design of chemicals-based products is broadly classified into those that are process centered and those that are product centered. In this article, the designs of both classes of products are reviewed from a process systems point of view; developments related to the design of the chemical product, its corresponding process, and its integration are highlighted. Although significant advances have been made in the development of systematic model-based techniques for process design (also for optimization, operation, and control), much work is needed to reach the same level for product design. Timeline diagrams illustrating key contributions in product design, process design, and integrated product-process design are presented. The search for novel, innovative, and sustainable solutions must be matched by consideration of issues related to the multidisciplinary nature of problems, the lack of data needed for model development, solution strategies that incorporate multiscale options, and reliability versus predictive power. The need for an integrated model-experiment-based design approach is discussed together with benefits of employing a systematic computer-aided framework with built-in design templates.

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**Phenomena Based Process Intensification of Toluene Methylation for Sustainable Para-xylene Production**

The objective of this work is to generate more sustainable intensified process designs for the production of important chemicals in the petrochemical sector. A 3-stage approach is applied. In stage 1, the base case design is generated or selected from literature. In stage 2, the base case design is analysed in terms of economics, sustainability and LCA factors in order to identify process hot-spots that are translated into design targets. In stage 3, intensified flowsheet alternatives are generated that match the targets and thereby eliminate and/or minimize the process hot-spots using a phenomena based method. Here, the flowsheet is decomposed into unit operations, tasks and phenomena that are analysed and selected in order to increase driving forces related to, for example, reaction and separation. The phenomena are then recombined to fulfil tasks that are translated into intensified unit operations to generate more sustainable designs. An overview of the key concepts and framework are presented together with the results from a case study highlighting the application of the framework to the sustainable design of a production process for para-xylene, which is an important chemical utilized in the production of polymers such as polyesters.

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Organisations: Department of Chemical and Biochemical Engineering, Chulalongkorn University
Predictive Modelling of Phase-Transfer Catalyst Systems for Improved and Innovative Design

Phase-transfer catalyst (PTC) systems contain two immiscible liquid phases with a heterogeneous PTC transferring active ion from one phase to the other for converting the reactant to the desired product, and in the process generating the inactive ion. This type of reacting systems is receiving increasing attention as a novel organic synthesis option due to its flexible and easier operation, higher production yield, and ability to eliminate expensive solvents, although, not eliminating the use of solvents.

New mathematical models of the PTC system, which includes physical and chemical equilibrium, reaction mechanism and unit operation has been developed. In the developed model, the PTC system is divided into four sub-systems of aqueous-organic solvent partition, inorganic salt in aqueous phase, PTC in aqueous phase, and PTC in aqueous phase. Each subsystem requires an appropriate thermodynamic model to predict the partition and equilibrium of the involved species. A new predictive electrolyte model (e-KT-UNIFAC) that has the capability to predict the partition and equilibrium of systems containing novel PTCs has been embedded into the reactor model. With this option, the application range has been significantly widened, making it feasible to identify new and innovative biphasic reaction options.

In this paper, the predictive qualities of the new model together with the improvements in the predicted design and operation of reaction with PTC systems are highlighted. Also, applications of problem-specific models for selecting improved design alternatives based on different design targets are presented.
Preface
This special issue of Computers & Chemical Engineering contains extended versions of selected papers from the joint event of the 12th International Symposium on Process Systems Engineering (PSE) and the 25th European Symposium on Computer Aided Process Engineering (ESCAPE) held in Copenhagen during 31 May to 4 June 2015. These papers were recommended by the International Programming Committee and constitute a representative sample of the invited plenary lectures, invited keynote lectures, and contributed papers.

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- Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
- ISI indexed (2012): ISI indexed yes
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- Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
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- BFI (2010): BFI-level 2
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- Scopus rating (2009): SJR 1.154 SNIP 2.166
- Web of Science (2009): Indexed yes
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This paper reviews issues and applications for design of sustainable carbon dioxide conversion processes, specifically through chemical conversion, and the integration of the conversion processes with other systems from a process systems engineering (PSE) viewpoint. Systematic and computer-aided methods and tools for reaction network generation, processing route generation, process design/optimization, and sustainability analysis are reviewed with respect to carbon dioxide conversion. Also, the relevant gaps and opportunities are highlighted. In addition, the integration of carbon dioxide conversion processes with other systems including coexisting infrastructure and carbon dioxide sources is described. Then, the importance of PSE based studies for such application is discussed. Finally, some perspectives on the status and future directions of carbon dioxide conversion technology and the development and use of PSE approaches are given.
Property Model-based Tailor-made Design of Chemical-based Products

Computer-aided model-based methods and tools are increasingly playing important roles in chemical product design. They have the potential to very quickly search for and identify reliable product candidates that can then be verified through experiments. In this way, the time and resources spent on experiment are reduced leading to faster and cheaper to market the products. The tools also help to manage the solution of product design problems, which usually require efficient handling of model-data-knowledge from different sources and at different time and size scales.

The main contribution of this project is: (1) the development of a systematic model-based framework for chemical product design; (2) its implementation as a computer-aided tool based on a specially developed architecture; (3) the creation of product design template together with their algorithms, models, tools and data for various types of products. The goal has been to develop a chemical product simulator, similar in concept to a process simulator, which make the product design and development easier and faster, and provide the way for unified and consistent product documentation. In the same way a typical process simulator works, the developed product simulator (VPPD-Lab) allows product designers to: (1) analyze chemicals based products by performing virtual experiments (product property and performance calculations); (2) predict the properties of products; and (3) create new product property and product performance models, when needed. However, unlike process simulators, VPPD-Lab can also be used directly for (4) design of chemicals based products using
the design template for various types of products, such as, single molecule products, formulations, blends, emulsions and devices; and, (5) creation of new product design templates when the needed template for a desired product is not available. VPPD-Lab employs a suite of algorithms (such as database search, molecular and mixture blend design) and toolboxes (such as property calculations and property model consistency tests) for specific product property prediction, design, and/or analysis tasks.

In order to achieve the features mentioned above, several issues need to be addressed: the translation of consumer needs into target properties; property models and available data for each type of chemical products; design methods and algorithms; available computer-aided tools; the systematic framework for chemical product design and analysis and its implementation as architecture for VPPD-Lab. From many test problems, eight application examples are presented to illustrate the use of the software. For two of these examples, the prediction of product properties and the use of virtual experiments to test product performances are highlighted. Five examples illustrate the use of the product design templates with respect to five types of chemical products (molecular design, formulation design, emulsion design, blend design and device design).

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Solvent selection methodology for pharmaceutical processes: Solvent swap
A method for the selection of appropriate solvents for the solvent swap task in pharmaceutical processes has been developed. This solvent swap method is based on the solvent selection method of Gani et al. (2006) and considers additional selection criteria such as boiling point difference, volatility difference, VLE phase diagram analysis, and azeotropic information that are particularly important for the solvent swap task. The method employs a solvent-swap database together with calculation tools for properties–functions of solvents. The database contains solvents that are commonly used in pharmaceutical processes as well as new solvent swap alternatives. The method takes into account process considerations such as batch distillation and crystallization to achieve the swap task. Rigorous model based simulations of the swap operation are performed to evaluate and compare the performance of the selected solvents. A guide and a software tool that allow the fast and reliable identification of the swap solvent have been developed. The main features and the applicability of the method are highlighted through several practical examples.

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Sustainable Chemical Process Development through an Integrated Framework

This paper describes the development and the application of a general integrated framework based on systematic model-based methods and computer-aided tools with the objective to achieve more sustainable process designs and to improve the process understanding. The developed framework can be applied to a wide range of problems, including the design of new processes as well as retrofit of existing batch-continuous production systems. The overview of the framework
together with results from two case studies is presented to highlight the key aspects and the applicability of the framework. These case studies involve multiphase reaction systems for the synthesis of active pharmaceutical ingredients.

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**Sustainable DME synthesis-design with CO2 utilization**
Minimizing CO2 emission, while achieving economic feasibility in CO2 utilization for producing valuable chemicals is a challenging problem, as reported in recent studies. Due to its high Cetane number, clean-burning, and non-toxic, DME is a promising fuel alternative, and therefore, potentially valuable chemical that can be produced via thermochemical CO2 conversion reactions. The aim of this study is to identify the most promising processing route for sustainable production of DME in terms of CO2 emission, economic indicators and sustainable indicators. The three processing routes are generated: (A) dry reforming step, methanol synthesis step, and methanoldehydration step; (B) CO2 hydrogenation step followed by methanol dehydration step; and (C) dry reforming step followed by direct DME synthesis step. Starting with a base-case design, the process flow sheets for the three routes are studied in detail to identify the process bottlenecks or hot-spots. Alternatives addressing the hot-spots are generated to identify the processing route with the best potential. The results indicate that processing route-B gives the highest CO2 consumption; nevertheless, this route is not feasible in terms of economic factors due to the negative rate of return. The final selection, however, depends on a trade-off between CO2 consumption and economic sustainability indicators. In principle, for all three alternatives are more sustainable options.

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**Sustainable DME synthesis-design with CO2 utilization**
Minimizing CO2 emission, while achieving economic feasibility in CO2 utilization for producing valuable chemicals is a challenging problem, as reported in recent studies. Due to its high Cetane number, clean-burning, and non-toxic, DME is a promising fuel alternative, and therefore, potentially valuable chemical that can be produced via thermochemical CO2
conversion reactions. The aim of this study is to identify the most promising processing route for sustainable production of DME in terms of CO2 emission, economic indicators and sustainable indicators. The three processing routes are generated: (A) dry reforming step, methanol synthesis step, and methanol dehydration step; (B) CO2 hydrogenation step followed by methanol dehydration step; and (C) dry reforming step followed by direct DME synthesis step. Starting with a base-case design, the process flow sheets for the three routes are studied in detail to identify the process bottlenecks or hot-spots. Alternatives addressing the hot-spots are generated to identify the processing route with the best potential. The results indicate that processing route-B gives the highest CO2 consumption; nevertheless, this route is not feasible in terms of economic factors due to the negative rate of return. The final selection, however, depends on a trade-off between CO2 consumption and economic-sustainability indicators. In principle, for all three alternatives are more sustainable options.

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**Sustainable process design & analysis of hybrid separations**

Distillation is an energy intensive operation in chemical process industries. There are around 40,000 distillation columns in operation in the US, requiring approximately 40% of the total energy consumption in US chemical process industries. However, analysis of separations by distillation has shown that more than 50% of energy is spent in purifying the last 5-10% of the distillate product. Membrane modules on the other hand can achieve high purity separations at lower energy costs, but if the flux is high, it requires large membrane area. A hybrid scheme where distillation and membrane modules are combined such that each operates at its highest efficiency, has the potential for significant energy reduction without significant increase of capital costs. This paper presents a method for sustainable design of hybrid distillation-membrane schemes with guaranteed reduction of energy consumption together with two illustrative examples.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, University of Kansas
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Systematic, efficient and consistent LCA calculations for chemical and biochemical processes

Life Cycle Assessment or LCA is a technique, which is applied for the study and evaluation of quantitative environmental impacts through the entire life cycle of products, processes or services in order to improve and/or evaluate the design of existing as well as new processes. The LCA factors can be used to identify and to improve the process environmental hotspots in order to make the process more sustainable. To complete the sustainable development of a process design, it is therefore necessary to consider both economic and environmental aspects. For this purpose, the LCSoft, a tool for systematic and consistent calculation of LCA factors has been developed (Supawanich et al., 2015). LCSoft integrates with other tools such as process simulation (PROII/ASPEN), ECON (economic analysis) and SustainPro (sustainability analysis) and provides for a specified boundary, all the established LCA factors. In this paper, new features that have widened the application range of LCSoft are presented together with evaluation of their performance. More specifically, this research focuses on improvements of the software performance in terms of extension of the LCI database and new calculation options that allow a wider coverage of chemical and biochemical processes. Improvements of LCIA calculations and eco-efficiency evaluation are introduced. Also, a new model for photochemical ozone formation has been developed and implemented. Performance of LCSoft in terms of accuracy and reliability is compared with another well-known LCA-software, SimaPro for a biochemical process – the production of bioethanol from cassava rhizome. The results show a very good match of new added impact categories. Also, the results from a new feature in LCSoft, which is eco-efficiency evaluation, are presented.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Chulalongkorn University
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Systematic framework for carbon dioxide capture and utilization processes to reduce the global carbon dioxide emissions

In the year 2013, 9.5 billion metric tons of carbon dioxide gas was emitted into the air, and each year this amount is increasing [1]. Carbon dioxide emissions are of particular concern as they represent 80% of greenhouse gas emissions and therefore are a large contributor to global warming. Among the two approaches that are currently being investigated, carbon capture and storage (CCS) and carbon capture and utilization (CCU) [1] to address this issue, the later approach is more promising as it reuses captured carbon dioxide, as a fuel, reactant, solvent, and others, to produce valuable products. There is not only a need for technologies for capture and utilization, via conversion, but also there are numerous questions that need to be resolved. For example, which higher value chemicals can be produced, what are their current demands and costs of production, and, how much of the captured carbon dioxide would be utilized? Also, how much carbon dioxide would be indirectly generated due to the capture and utilization efforts? Can the regulated carbon dioxide emission reduction targets be achieved only through the CCU and/or CCS efforts? Therefore, there is a need for a systematic computer-aided framework through which the issue of global carbon dioxide emissions can be investigated in terms of different available capture-utilization technologies, solution methods, and benefit scenarios, with the objective to determine more sustainable solutions within an appropriate application boundary. The framework would need to provide, amongst other options: useful data from in-house databases on carbon dioxide emission sources; mathematical models from a library of process-property models; numerical solvers from library of implemented solvers; and, work-flows and data-flows for different benefit scenarios to be investigated.

It is useful to start by developing a prototype framework and then augmenting its application range by increasing the contents of its databases, libraries and work-flows and data-flows. The objective is to present such a prototype framework with its implemented database containing collected information-data on various carbon dioxide emission sources and available capture-utilization technologies; the model and solution libraries [2]; and the generic 3-stage approach for determining more sustainable solutions [3] through superstructure (processing networks) based optimization – adopted for
global carbon dioxide emission problems. More specifically, the prototype framework and the three-stage approach adopted for systematic and sustainable design of carbon capture and utilization processes incorporates (i) process synthesis stage, the determination of a processing path from a network of alternatives; (ii) process design, the design and analysis of a process or generated processing path in terms of process “hot-spots” or deficiencies to set design targets for improvement; and (iii) innovative and more sustainable design, determination of solutions matching the design targets. In this way, the starting point is an analysis of the current carbon dioxide emission status and the end point is an analysis of the more sustainable solutions in terms of one or more carbon dioxide benefit scenarios.

The developed framework contains a database constructed based on a developed knowledge representation structure, which has collected data on carbon dioxide emission sources, capture technologies, carbon dioxide-based reaction paths, and known utilization technologies leading to various products. The database currently has 5 carbon dioxide emission sources, 3 capture technologies, 10 conversion routes leading to 8 products, and over 50 reaction paths for many more products. The framework also integrates a software tool (the Super-O interface [2]) containing a library of process models and links to numerical solvers that enables the generation of processing networks (superstructure) and the determination of the optimal processing route. Finally, the framework has access to, a collection of tools for analysis, such as economic analysis, sustainability and life cycle assessment, and links to detailed process simulation (process simulators).

Following the work-flow and data-flow implemented in the framework, data for the carbon capture and utilization alternatives are retrieved from the database and linked to form a network using the interface tool, Super-O. For each alternative, models for economic and environmental impacts are available; the promising utilization products considered are methanol, dimethyl carbonate, and succinic acid. The optimal utilization process (or processes) is determined via a superstructure-based method (using solvers in GAMS). Then, the carbon dioxide emission values for the utilization routes are compared with the current industrial production routes for the listed products in order to identify those that have zero or negative emission values (objective function). Subsequently, the identified utilization processes are designed rigorously and further improved with unique technology and integration options. Using this approach, the utilization processes for methanol, dimethyl carbonate and succinic acid give the following interesting result: by converting at least 70% (methanol), 40% (dimethyl carbonate) and 20% (succinic acid) of the current industrial processes to the corresponding utilization processes, the emissions from these processes can be neutralized, representing over 100 million metric tons of emissions that are neutralized. Note that the issue of product demand increase has not been considered. Also, on a global scale, this reduction of carbon dioxide emissions represents a very small but very valuable reduction. A more complete sustainability analysis is needed to enlarge the boundary of the analysis; for example, the boundary can change in terms of reduction of non-renewable resources and the use of renewable energy sources, as well as more efficient and sustainable designs of current production routes. While a combination of methods is needed to globally address carbon dioxide emissions and other aspects of sustainability, this systematic approach to designing carbon capture and utilization processes shows the capacity for such processes to reduce emissions and improve sustainability while producing valuable products. The current prototype framework with its implemented methods and tools is a small but important step.

Collaboration and integration of data, methods and tools is necessary to provide a more sustainable solution to the global carbon dioxide emission problem.

**General information**

State: Published

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**Systematic Integrated Process Design and Control of Binary Element Reactive Distillation Processes**

In this work, integrated process design and control of reactive distillation processes is considered through a computer-aided framework. First, a set of simple design methods for reactive distillation column that are similar in concept to non-reactive distillation design methods are extended to design-control of reactive distillation columns. These methods are based on the element concept where the reacting system of compounds is represented as elements. When only two elements are needed to represent the reacting system of more than two compounds, a binary element system is identified. It is shown that the same design-control principles that apply to a non-reacting binary system of compounds are also valid for a reactive binary system of elements for distillation columns. Application of this framework shows that designing the reactive distillation process at the maximum driving force results in a feasible and reliable design of the process as well as the controller structure.

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In this work, integrated process design and control of reactive distillation processes that involve multiple elements (more than two) is addressed through a computer-aided hierarchical decomposition-based framework. Multiple elements are encountered for reactive systems when four or more compounds (including inert compounds) are encountered. The reactive distillation design methods and tools which are similar in concept to design of binary non-reactive distillations and binary reactive distillations are used for design of multi-element reactive distillation processes, such as driving force approach. The methods that are used in this work are based on equivalent binary element concept. This concept provides the representation of a multi-element system in terms of two key elements, light key and heavy key elements. First, the reactive distillation column is designed using the equivalent binary element driving force approach. Next, through analytical, steady-state and closed-loop dynamic analysis it is verified that the control structure, disturbance rejection and energy requirement of the reactive distillation column is better than any other operation point that is not at the maximum driving force. Furthermore, it is shown that the design at the maximum driving force can be both controlled using simple controllers such as PI as well as advanced controllers such as MPC.
Systematic methods and tools for design of sustainable chemical processes for CO₂ utilization

A systematic computer-aided framework for sustainable process design is presented together with its application to the synthesis and generation of processing networks for dimethyl carbonate (DMC) production with CO₂ utilization. The framework integrated with various methods, tools, algorithms and databases is based on a combined process synthesis-design-intensification method. The method consists of three stages. The synthesis-stage involves superstructure based optimization to identify promising networks that convert a given set of raw materials to a desired set of products. The design-stage involves selection and analysis of the identified networks as a base case design in terms of operational feasibility, economics, life cycle assessment factors and sustainability measures, which are employed to establish targets for improvement in the next-stage. The innovation-stage involves generation and screening of the more sustainable alternatives through a phenomena-based process intensification method. Applications of the framework are highlighted for the DMC production process.

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- Scopus rating (2001): SJR 0.955 SNIP 0.728
- Web of Science (2001): Indexed yes
- Scopus rating (2000): SJR 1.366 SNIP 1.025
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Systematic screening methodology and energy efficient design of ionic liquid-based separation processes

A systematic methodology for the screening of ionic liquids (ILs) as entrainers and for the design of ILs-based separation processes in various homogeneous binary azeotropic mixtures has been developed. The methodology focuses on the homogeneous binary aqueous azeotropic systems (for example, water+alcohols). Additionally, a Hildebrand solubility parameter group contribution model for ILs, and ILs miscibility database have been developed to screen the miscibility of the ILs with the target solute component and these parameters are considered as the main criteria for the screening of ILs. ILs were further screened based on a combination of criteria such as stability, toxicity, and their environmental impacts. All best ILs were used as entrainers, and an extractive distillation column (EDC) and ionic liquid recovery column were designed and simulated with a process simulator to determine the overall energy consumption of the ILs-based separation processes. Among all candidates, the best IL was selected based on the minimum energy requirement obtained from the simulation. Finally, the modification of the separation process to obtain design flexibility for other azeotropic series with respect to the change in size of the target solute was investigated using the same separation process and IL entrainer to obtain the same product purity. The proposed methodology has been evaluated through a case study of binary alcoholic aqueous azeotropic separation: water+ethanol and water+isopropanol.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Chulalongkorn University
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Toward the Development and Deployment of Large-Scale Carbon Dioxide Capture and Conversion Processes

In light of the depletion of fossil fuels and the increased daily requirements for liquid fuels and chemicals, CO2 should indeed be regarded as a valuable C-1. additional feedstock for sustainable manufacturing of liquid fuels and chemicals. Development and deployment of CO2 capture and chemical conversion processes are among the grand challenges faced by today's scientists and engineers. Very few of the reported CO2 capture and conversion technologies have been employed for industrial installations on a large scale, where high-efficiency, cost/energy-effectiveness, and environmental friendliness are three keys factors. The CO2 capture technologies from stationary sources and ambient air based on solvents, solid sorbents, and membranes are discussed first. Transforming CO2 to liquid fuels and chemicals, which are presently produced from petroleum, through thermochemical, electrochemical, photochemical, and biochemical routes are discussed next. The relevant state-of-the-art computational methods and tools as a complement to experiments are also briefly discussed. Finally, after pointing out the advantages and disadvantages of the currently available technologies for CO2 capture and conversion, ideas and perspectives for the development of new techniques, opportunities, and challenges are highlighted.

General information
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Water consumption in the energy sector

Energy, water, and food systems are closely interlinked in the Energy-Water-Food Nexus. Water is of paramount importance for the energy sector. Fossil fuels require water for extraction, transport and processing. Thermal power plants require water for cooling, whether they use nuclear, fossil or biofuels. Hydropower is based on water in rivers or reservoirs. Feedstock production for biofuels may depend on water for irrigation. On the other hand, energy is necessary for pumping of ground- and surface water, for water treatment as well as for transport and distribution of water to end-users. The waste water is often returned to the environment after energy requiring waste water management.

A Method for Sustainable Carbon Dioxide Utilization Process Synthesis and Design

As a result of increasing regulations and concern about the impact of greenhouse gases on the environment, carbon dioxide (CO₂) emissions are a primary focus for reducing emissions and improving global sustainability. One method to achieve reduced emissions, is the conversion of CO₂ to useful compounds via chemical reactions. However, conversion is still in its infancy and requires work for implementation at an industrial level. One aspect of this is the development of a methodology for the formulation and optimization of sustainable conversion processes. This methodology follows three stages for the process synthesis, design and more sustainable design. Using a superstructure-based approach a network of utilization alternatives is created linking CO₂ and other raw materials with various products using processing blocks. This will then be optimized and verified for sustainability. Detailed design has also been performed for various case studies. These case studies include multiple pathways for the production of methanol and the production of dimethyl carbonate (DMC). From detailed design and analysis, CO₂ conversion processes show promise as an additional method for the sustainable reduction of CO₂ emissions.
A Methodology for a Sustainable CO2 Capture and Utilization Network

Climate change is a global issue that has come to the forefront of environmental concern. With the increasing emissions of greenhouse gases, efforts have increased to reduce carbon dioxide (CO2) emissions. Regulatory guidelines are becoming more stringent and efforts for long-term reduction are being investigated and implemented [1]. Carbon Capture and Storage (CCS) is the dominant method that is discussed. However, CO2 utilization is receiving increased attention for its ability to help in long-term CO2 reduction and the formation of various chemical products. One of the primary elements of utilization is the conversion of CO2 to valuable products via chemical reactions with other raw materials. In order for this to be implemented at a large and industrial level, further work is necessary. As part of this, the work focuses on the formulation and design of a CO2 utilization network via a superstructure-based methodology.

The method developed involves three stages: a process synthesis stage, a design stage and an innovation stage. Following a superstructure based approach, a network of conversion processes is created. This network links CO2 and products through various processing blocks. Each processing block within the developed network needs to be mathematically described for optimization. The second stage is the detailed design of a path within the network, followed by analysis and improvement by creating a more sustainable design in the innovation stage. An additional element is the sustainable linkage of carbon capture to produce the CO2 feed and the subsequent conversion processes. A manipulation of an MEA absorption process, the current industrial standard for carbon capture [2], is investigated. The resulting CO2 stream can be directly fed into a variety of conversion processes.

However, as not all information is available to describe the network mathematically, the most promising paths based on known technologies are designed and analyzed first. This makes the stages iterative rather than purely sequential. As part of this, a conceptual example of methanol synthesis via CO2 hydrogenation highlights the application. This case study illustrates the utility of the utilization network and elements of the methodology being developed. In addition, the conversion process is linked with carbon capture to evaluate the overall sustainability. Finally, the production of the other raw materials is also analyzed for economic feasibility and environmental sustainability. Using computer-aided methods, the feasibility and sustainability of CO2 conversion is shown through the design and optimization of a methanol synthesis process.

References:
A Model-Based Methodology for Integrated Design and Operation of Reactive Distillation Processes

Process intensification is a new approach that has the potential to improve existing processes as well as new designs of processes to achieve more profitable and sustainable production. However, many issues with respect to their implementation and operation is not clear; for example, the question of operability and controllability. Traditionally process design and process control are considered as independent problems and are solved sequentially. The process design problem is usually solved to achieve the design objectives, and then, the operability and process control issues are identified, analyzed and resolved. A new approach is to tackle process intensification and controllability issues in an integrated manner, in the early stages of process design. This integrated and simultaneous synthesis approach provides optimal operation and more efficient control of complex intensified systems that suffice the process design objectives. Furthermore, it may also suggest innovative process alternatives which are more economical and environmentally sustainable. In this work, a systematic model-based methodology for integrated design and operation of reactive distillation operations is presented. Issues related to operation are addressed to ensure a stable and reliable process design at predefined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions. The methodology employs a decomposition-based method so that the complexity of the problems is reduced into a set of sub-problems that are solved sequentially. The method consists of four hierarchical stages: (1) pre-analysis, (2) steady state analysis, (3) dynamic analysis, and (4) evaluation stage. To illustrate the application of the proposed methodology, production of methyl-tert-butyl-ether (MTBE) using a reactive distillation column (RDC) is considered. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used. The methods are based on the element concept, which is used to translate a ternary system of compounds (methanol, isobutene and MTBE) to a binary system of elements (elements A and B). For a binary element system, a simple reactive McCabe-Thiele-type method (to determine the number of reactive stages) has been used. The reactive equilibrium curve is constructed through sequential calculation of reactive bubble points. For an energy-efficient design, the driving-force approach (to determine the optimal feed location) for a reactive system has been employed. For both thereactive McCabe-Thiele and driving force method, vapor-liquid equilibrium data are based on elements. Thereactive bubble point algorithm is used to compute the reactive vapor-liquid equilibrium data set. The operation of the RDC at the highest driving force and other candidate points is compared through openloop and closed-loop analysis. By application of this methodology it is shown that designing the process at the maximum driving force results in an energy efficient and operable design. It is verified that the reactive distillation design option is less sensitive to the disturbances in the feed at the highest driving force and has the inherent ability to reject disturbances.

General information
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Analysis and prediction of the alpha-function parameters used in cubic equations of state
The performance of two generalized alpha functions (Soave and generalized Twu functions requiring the acentric factor as input parameter) and two parameterizable alpha functions (Mathias-Copeman and Twu) incorporated in cubic equations of state (Redlich-Kwong and Peng-Robinson) are evaluated and compared regarding their ability to reproduce vapor pressure, heat of vaporization, liquid heat capacity, liquid density and second virial coefficient data. To reach this objective, extensive databanks of alpha function parameters were created. In particular, pitfalls of Twu-type alpha functions were evidenced and fixed. A new class of purely predictive alpha functions was derived by applying group-contribution (GC) methods to the prediction of alpha function parameters. The interest of such an approach is discussed and compared to another predictive approach (use of generalized alpha functions coupled with GC methods to predict the acentric factor)
A New Optimization Model for Computer-Aided Molecular Design Problems

Computer-Aided Molecular Design (CAMD) is a method to design molecules with desired properties. That is, through CAMD, it is possible to generate molecules that match a specified set of target properties. CAMD has attracted much attention in recent years due to its ability to design novel as well as known molecules with desired properties. The attention is in particular targeted at the design of chemical based products, such as solvents, refrigerants, active pharmaceutical ingredients, polymers, surfactants, lubricants, and more [1]. Property prediction methods are needed in molecular design, as they enable the prediction of the target properties of the generated candidate molecules from their structural information. Here, CAMD methods can be regarded as the reverse engineering approach to property prediction, as the target properties are known while the molecules that match them need to be determined. In this way, CAMD problems can be formulated as a Mixed Integer Linear/Non-Linear Program (MILP/MINLP). With the advent of connectivity-based prediction methods, several researchers have developed new strategies for embedding it with CAMD method. Constantinou et al. [2] proposed a systematic strategy for generating isomers from a set of groups. Harper et al. [3] proposed a framework for CAMD method, where the pre-design phase defines the basic needs, the design phase determines the feasible candidates (generates molecules and tests for desired properties) and the post-design phase performs higher level analysis of the molecular structure and the final selection of the product. Samudra and Sahinidis [4] proposed a new optimization model using relaxed property targets and refined property targets with structural corrections. It is usually difficult to model and solve the MILP/MINLP problem with structure information considered due to the increased size of the mathematical problem and number of alternatives. Thus, decomposition-based approach is proposed to solve the problem. In this approach, only first-order groups are considered in the first step to obtain the building block of the designed molecule, then the property model is refined with second-order groups based on the results of the first step. However, this may result in the possibility of an optimal solution being excluded. Samudra and Sahinidis [4] used property relaxation method in the first step to avoid this situation, but it is not always easy for the users to find the appropriate relaxations. On the other hand, the feasible region of the optimization problem will become larger when relaxations are applied, which makes the solution of the problem harder. In this paper, a new model for CAMD problems is proposed. The model has been developed for the consideration of higher order groups in the molecular generation step of CAMD through mathematical optimization [5]. The model can consider both first and second order groups simultaneously in the MILP/MINLP formulation through a set of mathematical constraints. Structural constraints are defined through a set of linear mathematical equations for the feasible generation of molecules and the connectivity of molecular groups through the adjacency matrix. Property constraints are defined from a set of linear constraints based on the group contribution method [2]. The structural information of the molecule is obtained from the solution of the adjacency matrix. The adjacency matrix provides the adjacent connectivity of first order molecular groups. From this, the second order group description is found, which increases the structural information and property prediction accuracy. This will avoid the possible situation in which the optimal point is excluded from the feasible region due to inaccurate property prediction and ensures the obtainability of a global optimal solution. The model is implemented into a GAMS-based environment for the efficient optimization of a given problem. The model applicability will be demonstrated through the solution of a range of product design problems from literature, such as design of simple molecules (solvents and refrigerants) to design of complex molecules (polymers, lipids and surfactants).
An Integrated, Multi-Stage, Multi-Scale Framework for Achieving Sustainable Process Synthesis-Intensification-Control

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

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

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

In this presentation, the integrated process synthesis-intensification-control framework will be presented together with the corresponding databases, computer-aided models and tools needed to achieve sustainable synthesis-intensification. Different examples, related to synthesis, intensification and control will be presented for each stage of the framework.
Application of CAPEC Lipid Property Databases in the Synthesis and Design of Biorefinery Networks

Petroleum is currently the primary raw material for the production of fuels and chemicals. Consequently, our society is highly dependent on fossil non-renewable resources. However, renewable raw materials are recently receiving increasing interest for the production of chemicals and fuels, so a new industrial system based on biomass, an inexpensive, abundant and renewable raw material, is being established with sustainability as the main driving force [1]. The processing facilities for the production of multiple products (including biofuels and chemicals) from biomass are referred as biorefineries [2]. The wide variety and complex nature of components in biorefineries poses a challenge with respect to the synthesis and design of these types of processes. Whereas physical and thermodynamic property data or models for petroleum-based processes are widely available, most data and models for biobased processes are not. Lipids are present in biorefinery processes: they represent feedstock (vegetable oil, waste cooking oil, microalgal oil), intermediate products (fatty acids, glycerol) and final products in biorefineries, thus the prediction of their properties is of relevance for the synthesis and design of biorefinery networks.

The objective of this work is to show the application of databases of physical and thermodynamic properties of lipid components to the synthesis and design of biorefinery networks.

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Application of New Electrolyte Model to Phase Transfer Catalyst (PTC) Systems

Abstract Phase transfer catalyst (PTC) is used to transfer the desirable active form of an anion from the aqueous phase to organic phase where the reaction occurs. One of major challenges for process design of the PTC system is to establish a reliable thermodynamic model capable of describing phase behaviours of all components including water, organic solvents, inorganic salts, and the PTC. In this work, a new electrolyte model based on the KT-UNIFAC group contribution approach has been developed by adding the Debye-Hückel theory and a second virial coefficient-type term into the KT-UNIFAC model. The temperature-dependent parameters of the new model are introduced to improve the description of phase equilibria in temperature ranges between 273.15 and 373.15 K. The proposed model has been successfully applied to the predictions of phase behaviours of alkali halide aqueous solutions that are usually found in PTC systems, thereby, extending the application range of the PTC-system model. The solubility of PTC in organic solvents, which is a key factor
for strategy of PTC and solvent selection, has been calculated using the e-NRTL-SAC model.

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**Assessment of Recent Process Analytical Technology (PAT) Trends: A Multi author Review**

This multi author review article aims to bring readers up to date with some of the current trends in the field of process analytical technology (PAT) by summarizing each aspect of the subject (sensor development, PAT based process monitoring and control methods) and presenting applications both in industrial laboratories and in manufacture e.g. at GSK, AstraZeneca and Roche. Furthermore, the paper discusses the PAT paradigm from the regulatory science perspective. Given the multidisciplinary nature of PAT, such an endeavour would be almost impossible for a single author, so the concept of a multi author review was born. Each section of the multi author review has been written by a single expert or group of experts with the aim to report on its own research results. This paper also serves as a comprehensive source of information on PAT topics for the novice reader.

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A Systematic Computer-Aided Framework for Integrated Design and Control of Chemical Processes

Chemical processes are conventionally designed through a sequential approach. In this sequential approach, first, a steady-state process design is obtained and then, control structure synthesis that, in most of the cases, is based on heuristics is performed. Therefore, process design and process control and operation considerations have been studied
independently. Furthermore, this sequential approach does not adequately answer this question, "How do process design decisions influence process control and operation?". In order to answer this question, it is necessary to consider process controllability and operability issues together with process design tasks (Seferlis and Georgiadis, 2004). In this way, it can be assured that design decisions give the optimum operational and economic performance. Operability issues are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions.

In this work, a systematic hierarchical computer-aided framework for integrated process design and control of chemical processes including process intensification is proposed. Note however, because of integration of functions/operations into one system the controllability region of intensified equipment may become smaller (Nikačević et al., 2012). The methodology developed in this work employs a decomposition-based approach so that the complexity of the problem is reduced into a set of sub-problems that are solved sequentially. The production of methy-tert-butyl-ether (MTBE) is used to demonstrate the application of the framework. First, optimal design-control solution is presented for MTBE production via a reactor-separator-recycle (RSR) system. Next, it will be shown that the RSR system can be replaced by an intensified unit operation, a reactive distillation column (RDC) which optimal design-control solution is also presented. The operation and control of the RSR and RDC at the optimal designs is compared with other candidate designs compared through open-loop and closed-loop analysis. By application of this methodology it is shown that the optimal design obtained from this methodology, it is not only the best from an economic steady-state design point of view, but also from control and operation point view. It is verified that the optimal design options for RSR and RDC are less sensitive to the disturbances in the feed at the optimal design.

**A Systematic Computer-Aided Framework for Integrated Design and Control of Chemical Processes**

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**A Systematic Modelling Framework for Phase Transfer Catalyst Systems**

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Refrigerants are widely used in household and industrial applications, such as processes for energy transfer from low grade heat sources. Refrigerants are utilized in heat pump cycles for moving heat from one source to another with the task to heat or to refrigerate. Environmental issues have been a driving force for the industry to continuously seek novel refrigerants as current refrigerants risk phasing out due to environmental regulations. This trend has been seen since the Kyoto Protocol in 1997 and recently from the EU regulations from 2014, which will restrict the use of some known refrigerants today (Mota-Babiloni et al., 2015). However, design of new refrigerants poses a great challenge and finding an optimum solution for a given application often faces trade-off issues between cycle performance and environmental criteria. In addition, following issues are still to be addressed. What target properties and needs should carefully be selected for a given heat pump cycle to ensure that an optimum refrigerant is found? How can cycle performance and
environmental criteria be integrated at the product design stage and not in post-design analysis? Computer-aided product design methods enable the possibility of designing novel molecules, mixtures and blends, such as refrigerants through a systematic framework (Cignitti et al., 2015; Yunus et al., 2014). In this presentation a computer-aided framework is presented for chemical product design through mathematical optimization. Here, molecules, mixtures and blends, are systematically designed through a decomposition based solution method. Given a problem definition, computer-aided molecular design (CAMD) problem is defined, which is formulated into a mixed integer nonlinear program (MINLP). The decomposed solution method then sequentially divides the MINLP into smaller sub-problems; (i) MILP for molecular structure generation, (ii) LP for pure property constraints, (iii) NLP for mixtureblend constraints, (iv) NLP for process constraints. With this, it is ensured that the MINLP is feasible to solve and that a global optimum is reachable. The method is applied on refrigerant design for a heat pump cycle. It is shown how the presented framework can generate optimal novel refrigerants that are high performing and environmentally friendly. This is achieved through integrated product-process based optimization objective, namely, target physicochemical and environmental properties for refrigerant design and target heat pump cycle performance.

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Computer-aided Framework for Design of Pure, Mixed and Blended Products
Design of novel chemical products with process and application considerations is an emerging topic in the field of chemical and biochemical engineering. Methods, such as Computer Aided Molecular Design (CAMD) [1] and Computer-aided Mixture and Blend Design (CAMbD) [2], provide the possibility of designing such products. However, these product design problems can quickly become large and difficult, if not infeasible, to solve through mathematical optimization. In addition, considerations of process, application, special product attributes, economic feasibility, environmental and sustainability metrics that must be included in today’s product designs, consequently makes the problem harder to mathematically formulate and to solve. In this work, a framework for computer-aided design of pure, mixed and blended chemical products has been developed. The framework is a systematic approach to formulate and solve CAMbD problems through four sequential steps. In the first step, the needs, target properties and product type are defined. In the second step, the CAMbD is formulated together with objectives and process/application model. In the third step, the formulation is then converted into a mixed integer non-linear program (MINLP). In step four, the MINLP is directly solved (if possible) or sequentially solved through a decomposed optimization approach. The decomposed approach can solve a large MINLP by decomposing it into a smaller set of sub-problems. The framework application is highlighted through a solvent design case study.

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Computer-aided Framework for Design of Pure, Mixed and Blended Products

This paper presents a framework for computer-aided design of pure, mixed and blended chemical based products. The framework is a systematic approach to convert a Computer-aided Molecular, Mixture and Blend Design (CAMbD) formulation, based on needs and target properties, into a mixed integer non-linear program (MINLP). The MINLP is sequentially solved through a decomposed optimization approach to solve the possibly large MINLP in a smaller set of sub-problems. The framework application is highlighted through a solvent design case study.

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Computer-aided modelling template: Concept and application

Modelling is an important enabling technology in modern chemical engineering applications. A template-based approach is presented in this work to facilitate the construction and documentation of the models and enable their maintenance for reuse in a wider application range. Based on a model decomposition technique which identifies generic steps and workflow involved, the computer-aided template concept has been developed. This concept is implemented as a software tool, which provides a user-friendly interface for following the workflow steps and guidance through the steps providing additional information and comments on model construction, storage and future use/reuse. The application of the tool is highlighted with a multi-scale modelling case study involving a catalytic membrane fixed bed reactor and a two-phase system for oxidation of unsaturated acid with hydrogen peroxide. Both case studies reflect different aspects of template creation and use with respect to model development.

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Computer-aided tool for solvent selection in pharmaceutical processes: Solvent swap

In the pharmaceutical processes, solvents have a multipurpose role since different solvents can be used in different stages (such as chemical reactions, separations and purification) in the multistage active pharmaceutical ingredients (APIs) production process. The solvent swap and selection tasks are important factors in API production. The solvent swap problem is defined as the process where a swap solvent is added to the original solvent solution and the original solvent finally is removed by distillation or liquid-liquid extraction. The selection of an appropriate solvent for each process step is usually based on experience where knowledge-based methods could be employed. However, because of economical, safety and environmental concerns, the use of solvent selection guides together with model-based verification is a better option. Gani et al. (2006) have proposed a computer-aided framework where the solvent selection problem can be solved considering all the concerns mentioned above. The solvent swap problem can be treated as a special solvent selection (Gani et al., 2006) problem together with additional criteria consideration, involving VLE (vapour–liquid equilibria) and LLE (liquid-liquid equilibria). The application of the developed model-based framework is highlighted through several cases studies published in the literature. In the current state, the framework is suitable for problems where the original solvent is exchanged by distillation. A solvent selection guide for fast of suitable swap solvents is developed and is used to retrieve information for the most commonly used solvent candidates typically found in the pharmaceutical industry. The selection is verified by simulation. The framework for the solvent selection and solvent swap is part of an integrated computer-aided framework with the objective to assist the pharmaceutical industry in gaining better process understanding. A software interface to improve the usability of the tool has been created also.

Design of a process template for amine synthesis

A conceptual nitro reduction process template that should be generic such that it can handle a series of substrates with similar molecular functionality has been designed. The reduction process is based on a continuous plug-flow slurry reactor. The process template aims at speeding up the process development for new substrates by being easily adapted for a range of substrates as well as easily scaled by numbering-up. The potential saving in process development time could make it a particularly powerful experimental tool for early delivery campaigns in the pharmaceutical industry for the production of Kg amounts of material for clinical trials.

Design of Separation Processes with Ionic Liquids

A systematic methodology for screening and designing of Ionic Liquid (IL)-based separation processes is proposed and demonstrated using several case studies of both aqueous and non-aqueous systems, for instance, ethanol + water, ethanol + hexane, benzene + hexane, and toluene + methylcyclohexane. The best four ILs of each mixture are [mmim][dmp], [emim][bti], [emim][tso4] and [hmim][tcb], respectively. All of them were used as entrainers in the extractive
distillation. A process simulation of each system was carried out and showed a lower both energy requirement and solvent usage as compared to conventional organic solvent process.

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

Formulation and Design of a CO2 Utilization Network Detailed Through a Conceptual Example

Climate change is a global issue that has come to the forefront of environmental concern. With the increasing emissions of greenhouse gases, efforts have increased to reduce carbon dioxide (CO2) emissions. Regulatory guidelines are becoming more stringent and efforts for long-term reduction are being investigated and implemented [1]. Carbon Capture and Storage (CCS) is the dominant method that is discussed. However, CO2 utilization is receiving increased attention for its ability to help in long-term CO2 reduction and the formation of various chemical products. One of the primary elements of utilization is the conversion of CO2 to valuable products via chemical reactions with other raw materials. In order for this to be implemented at a large and industrial level, further work is necessary. As part of this, the work focuses on the formulation and design of a CO2 utilization network via a superstructure-based methodology. The sustainability and feasibility of linking carbon capture and CO2 conversion is studied in detail in a case study. CCS is still under development and CO2 utilization is showing great promise as an additional method of combatting CO2 emissions [2]. The method developed involves three stages: a process synthesis stage, a design stage and an innovation stage. Following a superstructure based approach, a network of conversion processes is created. This network links CO2 and products through various processing blocks. The network also links carbon capture to ensure the sustainability. Each processing block within the developed network needs to be mathematically described for optimization. The second stage is the detailed design of a path within the network, followed by analysis and improvement by creating a more sustainable design in the innovation stage. However, as not all information is available to describe the network mathematically, the most promising paths based on known technologies are designed and analyzed first. This makes the stages iterative rather than purely sequential. As part of this, the network is analyzed in the conceptual example of methanol synthesis via CO2 hydrogenation. This case study illustrates the utility of the utilization network and elements of the methodology being developed. In addition, the conversion process is linked with carbon capture to evaluate the overall sustainability. Finally, the production of the other raw materials is also analyzed for economic feasibility and environmental sustainability. Using computer-aided methods, the feasibility and sustainability of CO2 conversion is shown through the design and optimization of a methanol synthesis process.
Formulation of a Network and the Study of Reaction Paths for the Sustainable Reduction of CO2 Emissions

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

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

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

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

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

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

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Industrial wastewater treatment network based on recycling and rerouting strategies for retrofit design schemes

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

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Process design and process control have been considered as independent problems for many years. In this context, a sequential approach is used where the process is designed first, followed by the control design. However, this sequential approach has its limitations related to dynamic constraint violations, for example, infeasible operating points, process overdesign or under-performance. Therefore, by using this approach, a robust performance is not always guaranteed.

**Integrated Design and Control of Reactive and Non-Reactive Distillation Processes**

Process design and process control have been considered as independent problems for many years. In this context, a sequential approach is used where the process is designed first, followed by the control design. However, this sequential approach has its limitations related to dynamic constraint violations, for example, infeasible operating points, process overdesign or under-performance. Therefore, by using this approach, a robust performance is not always guaranteed.
Furthermore, process design decisions can influence process control and operation (Huusom, 2015). To overcome these limitations, an alternative approach is to tackle process design and controllability issues simultaneously, in the early stages of process design. This simultaneous synthesis approach provides optimal/near optimal operation and more efficient control of conventional (non-reactive binary distillation columns) (Hamid et al., 2010) as well as complex chemical processes; for example, intensified processes such as reactive distillation (Mansouri et al., 2015). Most importantly, it identifies and eliminates potentially promising design alternatives that may have controllability problems later. To date, a number of methodologies have been proposed and applied on various problems to address the interactions between process design and control, and they range from optimization-based approaches to model-based methods (Sharifzadeh, 2013).

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

The operation of the non-reactive distillation column, ternary reactive distillation column (binary-element) and multicomponent reactive distillation column (binary-key-element) is investigated at the highest driving force and other candidate points. It is shown analytically and through rigorous dynamic process simulation (using ICAS process simulation software and Aspen Plus) for all three cases that the sensitivity of the system to the disturbances in the feed at the highest driving force is less than any other candidate point. By application of this approach, it is shown that designing the non-reactive and reactive distillation processes at the maximum driving force results in an optimal design in terms of controllability and operability as well as an optimal/near optimal design from an energy point of view. It is verified that the reactive distillation design option is less sensitive to disturbances.
In this work, integrated process design and control of reactive distillation processes is presented. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used, such as reactive McCabe-Thiele method and driving force approach. The methods are based on the element concept, which is used to translate a system of compounds into elements. The operation of the reactive distillation column at the highest driving force and other candidate points is analyzed through analytical solution as well as rigorous open-loop and closed-loop simulations. By application of this approach, it is shown that designing the reactive distillation process at the maximum driving force results in an optimal design in terms of controllability and operability. It is verified that the reactive distillation design option is less sensitive to the disturbances in the feed at the highest driving force and has the inherent ability to reject disturbances.
Life Cycle Assessment Studies of Chemical and Biochemical Processes through the new LCSoft Software-tool

Life Cycle Assessment or LCA is an effective tool for quantifying the potential environmental impacts of products, processes, or services in order to support the selection making of desired products and/or processes from different alternatives. For more sustainable process designs, technical requirements have to be evaluated together with environmental and economic aspects. The LCSoft software-tool has been developed to perform LCA as a stand-alone tool as well as integrated with other process design tools such as process simulation, economic analysis (ECON), and sustainable process design (SustainPro). An extended version of LCSoft is presented in this paper. The development work consists of four main tasks. The first task consists of the Life Cycle Inventory (LCI) calculation function. The second task deals with the extension of the Life Cycle Inventory database and improvement of the Life Cycle Impact Assessment calculation. The third task deals with analysis to investigate the contributions of processes, LCI results, and environmental impact results with respect to the production stage. Also, an uncertainty analysis is included to investigate the influence of uncertain parameters on the LCI assessment results. The fourth task has been added to validate and improve LCSoft by testing it against several case studies and compare the assessment results with other available tools.

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Method for innovative synthesis-design of chemical process flowsheets

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

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

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

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

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Modelling Template for the Development of the Process Flowsheet

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 contribution a general modelling framework for systematic model building through modelling templates, which supports the reuse of existing models via its tools integration and model import and export capabilities, is presented. Modelling templates in connection to other modelling tools within the modelling framework are forming 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 three main parts: 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. In this work, the integrated use of all three parts in the modelling framework is highlighted through a development of a simple flowsheet model. Initially the model equations are obtained from the tool for model generation and then transferred to model analysis tool. Further, based on this model, a modelling template is created, which is used later for the modelling of Williams-Otto plant. The main goal is a demonstration of the template reuse for the system with similar repetitive objects.

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On the Integration Role of Solvents in Process Synthesis-Design-Intensification: Application to DMC/MeOH separation
Solvents (mass separating agents) play an important role in separation-based processes. For example, consider the separation of an azeotropic mixture. If the azeotrope is not pressure dependent, then a feasible separation technique that can be employed for separation of the azeotrope is usually extractive distillation. In extractive distillation the solvent affects the relative volatility of the two key compounds to be separated. In other words, for a two column distillation sequence configuration, the lighter boiling compound is obtained as the top product of the first distillation column and the heavier boiling compound is obtained as the top product of the second distillation column where the solvent is recovered (for reuse and recycle).

Therefore, the solvent design problem can be defined as follows, given an azeotropic mixture to be separated into two pure streams that utilizes a mass separating agent, find the best (optimal or near-optimal) solvent candidate (or mixture) that can perform the separation subject to economic, environmental and thermo-physical property constraints. This design problem inherently is a mixed integer non-linear programming problem because the property-process models used can be linear, non-linear or a combination of both and, numerous solvents (or solvent mixtures) can in principle be selected (Lei et al., 2015).

In this work, the generation, screening and verification of the solvent candidate follows a three stage approach, in order to, decompose the solvent design problem into manageable sub-problems. In the first stage, a number of solvent candidates are generated based on pre-defined structural constraints, for example, acyclic, cyclic and/or aromatic compounds, etc. In the second stage, the solvent candidates are screened using property constraints, for example, temperature/temperature dependent properties and environmental properties. In stage 3, the selected feasible solvent candidates are
verified through simulation for selection of the best (optimal) solvent candidate (mixture). In stages 1-3, property models play an integration role, service plus advice role and service role respectively (Kontogeorgis and Gani, 2004). Application of the method is highlighted for a typical azeotropic mixture separation. Di-methyl carbonate (DMC) is an important chemical because it can be used as a fuel additive and is therefore considered to be one of the better replacements for methyl tert-butyl ether. Methanol (MeOH) is used as a common raw material in the production of DMC, for example, using phosgene with hydrochloric acid as the by-product, using carbon monoxide and oxygen with water as the by-product, using a cyclic carbonate with a glycol as the by-product, etc. Therefore, recovery/separation of MeOH/DMC is an important separation sequence encountered in generating more sustainable process alternatives for the production of DMC (Babi et al., 2015, Holtbruegge et al., 2014) using MeOH as the raw material. The objective of this presentation is to present the best separation system, with the focus on solvent generation, screening and verification for the separation of MeOH and DMC. The three stage approach will be presented and it will be shown that existing solvent candidates found in the literature are already generated in the “generation” stage plus new solvent candidates. In the “screening” and “verification” stages, it will be shown that two solvent candidates (not previously reported) are selected that satisfy the structural, property and environmental constraints for the effective separation and recovery of MeOH and DMC. Finally, a design of experiments method will be presented in order to cover the design and pilot testing of the best solvent candidate.

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

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Optimal processing pathway selection for microalgae-based biorefinery under uncertainty

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

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Preface

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In practice, chemical process synthesis-design involves identification of the processing route to reach a desired product from a specified set of raw materials, design of the operations involved in the processing route, the calculations of utility requirements, the calculations of waste and emission to the surrounding and many more. In terms of approaches to solve the synthesis-design problem three major lines of attack have emerged: (a) the knowledge based approach [1] which
relies on engineering knowledge & problem insights, (b) the optimization approach [2] which relies on the use of mathematical programming techniques, (c) hybrid approach which combine two or more approaches. D’Anterroches [3] proposed a group contribution based hybrid approach to solve the synthesis-design problem where, chemical process flowsheets could be synthesized in the same way as atoms or groups of atoms are synthesized to form molecules in computer-aided molecular design (CAMD) techniques [4]. The main idea here was to apply the principle of group-contribution approach from chemical property estimation to the synthesis and design of chemical process flowsheets. That is, use process-groups representing different unit operations (reactor, distillation, flash, crystallization, etc.), bonds representing streams and/or recycles, rules for chemical feasibility also representing process flowsheet feasibility and sum of group contributions representing the performance of the flowsheet. In the next stage, the design parameters for the operations of the high ranked flowsheets are established through reverse engineering approaches based on driving forces available for each operation. In the final stage, rigorous simulation is performed to validate the synthesis-design. Note that since the flowsheet is synthesized and the operations in the flowsheet designed to match a set of design targets, there are no iterations involved as the final flowsheet is among the best, if not the best. In this work, the flowsheet synthesis-design framework is expanded to include process-groups representing the unit operations from biochemical processes and new flowsheet property models to predict the environmental impact, process safety, product recovery and purity, which are employed to screen the generated alternatives. The extended framework implemented in the form of a computer-aided tool, ProCAFD will be highlighted through two case studies, one involving the synthesis of a chemical process flowsheet (the well-known Hydrodealkylation of toluene process) and another for a biochemical process (production of Bio-ethanol). In both cases, various process alternatives were generated quickly using the ProCAFD tool. The framework was able to generate not only the reported designs, but also various innovative designs, due to predictive nature of the methods used. The application-examples also focus on the use of SFILES notation system, developed specially for the process-group based synthesis-design method, to store and/or visualize the structural information of any process flowsheet represented by process-groups. As an extension, the SFILES notation is extended to store the process information through which representation of flowsheet alternatives for rigorous process simulation (for example, with an external process simulator) would be possible.
Product design - Molecules, devices, functional products, and formulated products

Chemical product design is a multidisciplinary and diverse subject. This article provides an overview of product design while focusing on product conceptualization. Four product types are considered - molecular products, formulated products, devices and functional products. For molecular products, computer-aided design tools are used to predict the physicochemical properties of single molecules and blends. For formulated products, an integrated experiment-modeling approach is used to generate the formula with the specified product attributes. For devices and functional products, conceptual product design is carried out by modeling the product based on thermodynamics, kinetics and transport processes, by performing experiments, and by decision making based on rule-based methods. The results are product specifications in terms of the type of ingredients, composition, and the structure, form, shape or configuration of the product.
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Superstructure-based optimization of biorefinery networks: Production of biodiesel
Petroleum is currently the primary raw material for the production of fuels and chemicals. Consequently, our society is highly dependent on fossil non-renewable resources. However, renewable raw materials are recently receiving increasing interest for the production of chemicals and fuels, so a new industrial system based on biomass, an inexpensive, abundant and renewable raw material, is being established with sustainability as the main driving force [1]. The processing facilities for the production of multiple products (including biofuels and chemicals) from biomass are referred as biorefineries [2]. The optimal synthesis of biorefinery networks problem is defined as: given a set of biomass derived feedstock and a set of desired final products and specifications, determine a flexible, sustainable and innovative processing network with the targets of minimum cost and sustainable development taking into account the available technologies, geographical location, future technological developments and global market changes.

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

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

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Sustainable Process Design under uncertainty analysis: targeting environmental indicators

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

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Sustainable process synthesis-intensification

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

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Synthesis and Design of a Sustainable CO2 Utilization Network

In response to increasing regulations and concern about the impact of greenhouse gases on the environment, carbon dioxide (CO2) emissions are targeted for reduction. One method is the conversion of CO2 to useful compounds via
chemical reactions. However, conversion is still in its infancy and requires work for implementation at an industrial level. One aspect of this is the development of a methodology for the formulation and optimization of sustainable conversion processes. This methodology follows three stages for the process synthesis, design and more sustainable design. Using a superstructure-based approach a network of utilization alternatives is created linking CO2 and other raw materials with various products using processing blocks. This will then be optimized and verified for sustainability. Detailed design has also been performed for a case study on the methanol synthesis processing block. CO2 conversion processes show promise as an additional method for the sustainable reduction of CO2 emissions.

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

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Synthesis of biorefinery networks using a superstructure optimization based approach

Petroleum is currently the primary raw material for the production of fuels and chemicals. Consequently, our society is highly dependent on fossil non-renewable resources. However, renewable raw materials are recently receiving increasing interest for the production of chemicals and fuels, so a new industrial system based on biomass, an inexpensive, abundant and renewable raw material, is being established with sustainability as the main driving force [1]. The processing facilities for the production of multiple products (including biofuels and chemicals) from biomass are referred as biorefineries [2]. The optimal synthesis of biorefinery networks problem is defined as: given a set of biomass derived feedstock and a set of desired final products and specifications, determine a flexible, sustainable and innovative processing network with the targets of minimum cost and sustainable development taking into account the available technologies, geographical location, future technological developments and global market changes. The problem of optimal design of biorefinery networks is solved in this work through three different stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. At the synthesis stage, the considered alternatives are represented in a superstructure, from which a mixed-integer linear or nonlinear programming (MILP or MINLP) problem is derived and solved in order to find the optimal processing network for a pre-defined objective function. Next, at the design stage, the selected processing network is simulated and analyzed and targets for improvement are identified. Finally, a more sustainable design is achieved at the innovation stage by generating innovative solutions that satisfy the targets from the design stage. This work is concerned with the first stage: the synthesis stage. Various biorefinery processing alternatives are represented in a superstructure and the associated data is collected and stored in a database. Once a specific biorefinery synthesis problem is formulated, the superstructure is reduced in order to include only the relevant alternatives. The superstructure is reduced based on constraints from the problem formulation, such as location or raw material. The reduced superstructure is then represented using mathematical models - the modelling approach by Quaglia et al. [3] is used - and solved to find the optimal network. The applicability of the proposed approach is shown through a practical case study for the production of valuable products (i.e. lysine and lactic acid) from sugarcane molasses; these alternatives are considered with respect to availability and demands in Mexico [4].

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

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

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Systematic Approach to Design Tailor Made Fuel Blends That Meets ASTM Standards

Blending of chemicals to design a tailor-made product for desired characteristics is a common practice in industry. Similarly, blending of liquid fuel is done to formulate a chemical mixture in liquid state that is stable in ambient conditions and has desired target fuel properties. Designing such tailor-made fuel is a challenging task which includes finding suitable chemicals and their compositions within the blend that meets the desired target fuel properties. In this study a computer aided model based technique “Mixed Integer Non-Linear Programming” (MINLP) was used to design the tailor made blends [1]. The main architecture in MINLP has four structures viz., (i) problem definition (ii) property model identification (iii) mixture blend design and (iv) model-based verification. These structures are further subdivided in to sub-problems and a decomposition based solution approach was adopted to solve them [2]. Two tailor-made liquid fuels viz., gasoline and model diesel were formulated by our collaborator at the Technical University of Denmark conducting the MINLP program [3]. Different set of target properties were calculated for each type of fuel in order to design a set of suitable blend. The target properties calculated for tailor-made gasoline were flash point (TF), Reid vapor pressure (RVP) and kinematic viscosity (\( \nu \)). Target properties calculated for tailor-made diesel were high heating value (HHV), dynamic viscosity (\( \eta \)), lethal concentration (-logLC50), weight percent of oxygen (WtO2), density (\( \rho \)) and Reid vapor pressure (RVP). Model gasoline blend (main ingredient) designed using MINLP, comprised of six different chemicals viz. n-pentane, n-heptane, iso-octane, 1-pentene, methyl cyclopentane and toluene in different volumetric ratios. Similarly, model diesel blend (main ingredient) designed using MINLP, comprised of seven n-paraffinic compounds viz., n-decane, n-undecane, n-dodecane, n-tetradecane, n-hexadecane, n-octadecane and n-eicosane in different volumetric ratios.

The paper is focused on the experimental verification of the properties of diesel and gasoline models (main ingredients), according to composition of computational model identified by our collaborator at DTU. The composition of blends was verified using Gas Chromatograph (GC) analysis and through a comparison of measured and theoretical densities. Following that, different fuel properties such as flash point, vapor pressure, and heat content were determined using analytical instruments according to their respective American Society for Testing and Materials (ASTM) standards. Most of the properties complied well with the industry standards. However, model gasoline had a comparatively low RVP. On the other hand, model diesel had a significantly higher cloud point and pour point than what is recommended. This deviation will have an impact on the cold flow properties of the fuels. For both fuels, different additives along with their composition have also been determined using the same computational model. These additives will be added to the main ingredient and the complete experimental analysis will be carried out. The work will be further continued to study the engine performance and emission characteristic of both types of fuel blends along with their additives. This would provide a more realistic approach to design tailor made fuels. Result of this study would provide a scientific approach for formulation of blended fuels and could be used as basis for tailor made blends.

Systematic Computer-Aided Framework for Sustainable Chemical Product Design

Computer-aided product design (CAPD) is a method for the generation and selection of novel pure, mixed and blended chemical products [1]. In CAPD, the chemical product is generated and selected based on defined structure, property and process/application constraints. Several challenges exist for CAPD, including the accuracy of the property estimation, molecular structure generation, inclusion of sustainability, process and application targets and needs in the problem formulation. CAPD has been widely utilized for the synthesis of several types of products, such as solvents, polymers, fuels and formulated products [2]. However, for product design problems where the process needs and sustainability possess demanding constraints, the complexity of the problem is increased as the relation between product property, sustainability and process criteria is difficult to mathematically define. In this work, a generic computer-aided framework for
chemical product design is presented through a systematic framework. A CAPD problem for the generation of novel pure, mixed and blended chemical products is formulated and solved through the application of four sequential steps. In step (1), the product design problem is defined together with the process and/or application boundaries. In step (2), the CAPD problem is formulated through property constraints for pure, mixed and blended products, process/application constraints and objective function. The property constraints are carefully selected for the thermo-physical property needs and the process/application needs. Process/application and property needs are connected through an analysis of the property influence on the process/application models and thermodynamic relations. The sustainability is considered through product and process/application performance, economics and environmental impact. In step (3), the CAPD formulation is converted into a mixed-integer nonlinear program (MINLP) by set-up of constraints, objective and boundaries defined in step (2). In step (4), the MINLP is solved through a decomposed approach [3]. The decomposed approach breaks down the MINLP problem into a sub-set of programs to manage the complexity: mixed-integer linear program (MILP) for molecular generation, linear program (LP) for property constraints, non-linear program (NLP) for mixture/blend property constraints, and NLP for process constraints and objective function. This approach ensures that the optimal chemical product can be found through systematic generation and screening of alternatives based on the problem definition. The framework is implemented into a GAMS-based tool. The application of the framework is demonstrated through sustainable working fluid design for a heat pump cycle. Working fluids used in heat pumps are continuously regulated due to the environmental issues, such as ozone depletion or global warming potential. Many of the currently used working fluids are soon to be phased out [4]. The design of novel working fluids is a challenging task as retro-fitting as well as re-designing demand increased sustainability and minimal trade-off with system performance. In the CAPD formulation, the product properties are related to the needs of heat pump cycle and its components through sensitivity analysis of the thermodynamic models and energy balances of the system. Furthermore, simple models are included for efficient assessment of the sustainability and design criteria of both the cycle and its components. It will be demonstrated that the working fluid product designed is optimal with respect to the sustainability and the heat pump cycle performance.

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

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

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

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BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.68
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Scopus rating (2014): CiteScore 4.92
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BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.59
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BFI (2012): BFI-level 1
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Use of operating windows for assessment of continuous plug flow slurry reactor

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, AstraZeneca
Authors: Singh, R. (Intern), Gregertsen, B. (Ekstern), Muller, F. (Ekstern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
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Vapour liquid equilibria of monocaprylin plus palmitic acid or methyl stearate at $P=(1.20 \text{ and } 2.50) \text{ kPa}$ by using DSC technique

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, State University of Campinas, Universidade Federal de Sao Paulo, Alfa Laval Copenhagen A/S
Authors: Cunico, L. P. (Intern), Damaceno, D. S. (Ekstern), Matricarde Falleiro, R. M. (Ekstern), Sarup, B. (Ekstern), Abildskov, J. (Intern), Ceriani, R. (Ekstern), Gani, R. (Intern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1 SNIP 1.163
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.252 SNIP 1.25 CiteScore 2.42
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.221 SNIP 1.181 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
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Scopus rating (2011): SJR 1.24 SNIP 1.307 CiteScore 2.44
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 1.218 SNIP 1.462
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.116 SNIP 1.355
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.414 SNIP 1.269
Scopus rating (2007): SJR 1.264 SNIP 1.176
Scopus rating (2006): SJR 1.116 SNIP 1.415
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.913 SNIP 1.277
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.847 SNIP 1.124
Scopus rating (2003): SJR 0.726 SNIP 0.986
Scopus rating (2002): SJR 0.712 SNIP 1.21
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.581 SNIP 0.984
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.741 SNIP 1.164
Scopus rating (1999): SJR 0.914 SNIP 1.163
VPPD Lab - The Chemical Product Simulator

In this paper, the development of a systematic model-based framework for product design, implemented in the new product design software called VPPD-Lab is presented. This framework employs its in-house knowledge-based system to design and evaluate chemical products. The built-in libraries of product performance models and product-chemical property models are used to evaluate different classes of product. The product classes are single molecular structure chemicals (lipids, solvents, aroma, etc.), blended products (gasoline, jet-fuels, lubricants, etc.), and emulsified product (hand wash, detergent, etc.). It has interface to identify workflow/data-flow for the inter-related activities between knowledge-based system and model-based calculation procedures to systematically, efficiently and robustly solve various types of product design-analysis problems. The application of the software is highlighted for the case study of tailor made design of jet-fuels. VPPD-Lab works in the same way as a typical process simulator. It enhances the future development of chemical product design.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, University at Qatar
Authors: Kalakul, S. (Intern), Hussain, R. (Ekstern), Elbashir, N. (Ekstern), Gani, R. (Intern)
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Achieving More Sustainable Designs through a Process Synthesis-Intensification Framework

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
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Achieving more sustainable solutions through process intensification

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern)
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Achieving more sustainable solutions through process intensification

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Achieving More Sustainable Solutions through Process Intensification

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Achieving more sustainable solutions through process intensifications

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern)
Publication date: 2014
A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design

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

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

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Handani, Z. B. (Intern), Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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An Integrated Methodology for Emulsified Formulated Product Design

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Gani, R. (Intern), Kontogeorgis, G. (Intern)
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An Integrated Systematic Framework to Assist the Development of Pharmaceutical Processes

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

In this work, a couple of applications of the template-based approach for model development are presented. The computer-aided template concept has been developed based on a model decomposition technique and has been implemented as a software tool, which provides a user-friendly interface for following the modelling workflow steps, guidance through the steps, as well as providing additional information and comments. The application of the tool is highlighted with two case studies: oxidation of unsaturated acid with hydrogen peroxide and modeling of a crystal lization operation for the paracetamol-ethanol system.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Fedorova, M. (Intern), Papadakis, E. (Intern), Meisler, K. T. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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DOIs:

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

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Fedorova, M. (Intern), Papadakis, E. (Intern), Meisler, K. T. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2014
A process synthesis-intensification framework for the development of sustainable membrane-based operations

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Handani, Z. B. (Intern), Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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A Simultaneous Optimization Approach for Synthesis and Design of Process and Water Networks

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Authors: Handani, Z. B. (Intern), Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

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

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

Physical and thermodynamic properties of pure components and their mixtures are the basic requirement for process design, simulation, and optimization. In the case of lipids, our previous works[1-3] have indicated a lack of experimental...
Consistent vapour-liquid equilibrium data containing lipids

Consistent physical and thermodynamic properties of pure components and their mixtures are important for process design, simulation, and optimization as well as for design of chemical based products. In the case of lipids, it was observed a lack of experimental data for pure compounds and also for their mixtures in open literature, what makes necessary the development of reliable predictive models based on limited data. To contribute to the missing data, measurements of isobaric vapour-liquid equilibrium (VLE) data of three binary mixtures at two different pressures were performed at State University of Campinas (UNICAMP – Brazil), using Differential Scanning Calorimetry (DSC) technique, i.e., monoacylglycerol + fatty acid (system 1), monoacylglycerol + fatty ester (system 2) and monoacylglycerol + glycerol (system 3). System 1 is relevant in the purification steps of the deodorizer distillates while systems 2 and 3 are relevant in the purification steps of biodiesel and bioglycerin. It should be highlighted that there is no such data in the open literature, not only for the specific compounds we selected but also for the combination of the classes of compounds considered in this work. Available thermodynamic consistency tests for TPx data were applied before performing parameter regressions for well-known thermodynamic models such as Wilson, NRTL, UNIQUAC and UNIFAC. In the pure compound consistency test (Qtest,5 of TDE program developed at NIST), the consistencies of the end-points (x=0 and 1) of the VLE data are considered by comparing these values with their pure compound vapor pressures. Van Ness test where also considered in this work (Qtest,1 of program TDE developed at NIST), that check how the measured data represent the thermodynamic models. Boiling temperatures and vapor phase compositions were calculated using Wilson, NRTL, UNIQUAC and original UNIFAC models. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC models. For solid-liquid equilibrium (SLE) data, new consistency tests have been developed [2]. Some of the developed tests were based in the quality tests proposed for VLE data by Kang et al. [4] and a methodology that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions are discussed. In this work, case studies considering the methodology proposed for SLE thermodynamic consistency tests and data from open literature and databases such as NIST-TDE®, DIPPR® and DECHEMA® are presented. The SLE consistency test and data evaluation is performed in a software containing option for data analysis, model analysis and parameter regression.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, State University of Campinas, Alfa Laval Copenhagen A/S, Korea University
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Publication date: 2014
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Consistent vapour-liquid equilibrium data containing lipids

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, State University of Campinas, Alfa Laval Copenhagen A/S
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Crystallization Kinetics within a Generic Modeling Framework
A new and extended version of a generic modeling framework for analysis and design of crystallization operations is presented. The new features of this framework are described, with focus on development, implementation, identification, and analysis of crystallization kinetic models. Issues related to the modeling of various kinetic phenomena like nucleation, growth, agglomeration, and breakage are discussed in terms of model forms, model parameters, their availability and/or estimation, and their selection and application for specific crystallization operational scenarios under study. The advantages of employing a well-structured model library for storage, use/reuse, and analysis of the kinetic models are highlighted. Examples illustrating the application of the modeling framework for kinetic model discrimination related to simulation of specific crystallization scenarios and for kinetic model parameter estimation are presented.
Development and analysis of the Original UNIFAC-CI model for prediction of vapor–liquid and solid–liquid equilibria

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

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

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

Editorial note for the Best Paper of 2012 Award

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
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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Authors: Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Synthesis and design of processing network, Capital budgeting, Mixed Integer Non Linear Programming, Financial optimization
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**Hybrid Distillation Schemes: Design, Analysis & Application**

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Babi, D. K. (Intern), Gani, R. (Intern)
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Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
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**Improving Prediction Capability of Modelling Framework for Biphasic Reaction System**

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

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**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
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Integration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process design

The sustainable future of the world challenges engineers to develop chemical process designs that are not only technically and economically feasible but also environmentally friendly. Life cycle assessment (LCA) is a tool for identifying and quantifying environmental impacts of the chemical product and/or the process that makes it. It can be used in conjunction with process simulation and economic analysis tools to evaluate the design of any existing and/or new chemical-biochemical process and to propose improvement options in order to arrive at the best design among various alternatives. Although there are several commercial LCA tools, there is still a need for a simple LCA software that can be integrated with process design tools. In this paper, a new LCA software, LCSoft, is developed for evaluation of chemical, petrochemical, and biochemical processes with options for integration with other process design tools such as sustainable design (SustainPro), economic analysis (ECON) and process simulation. The software framework contains four main tools: Tool-1 is for life cycle inventory (LCI) knowledge management that enables easy maintenance and future expansion of the LCI database; Tool-2 is for estimation of environmental impact characterization factors using group contribution(+) method (GC)(+) in order to calculate environmental impacts for a wide range of chemicals; Tool-3 performs LCA calculations based on a library of models; and, Tool-4 provides interfaces for integration with other tools. To test the software, a bioethanol production process using cassava rhizome is employed as a case study. Results from LCSoft highlight the estimated environmental performance in terms of various aspects such as carbon footprint, resource and energy consumptions, and various environmental impacts. (C) 2014 Elsevier Ltd. All rights reserved.

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Ionic-Liquid Based Separation of Azeotropic Mixtures

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

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Measurement of VLE data for binary lipids systems
Consistent physical and thermodynamic properties of pure components and their mixtures are important for process design, simulation, and optimization as well as design of chemical based products. In the case of lipids, our previous works[1-3] have indicated a lack of experimental data for pure components and also for their mixtures. To contribute in this area, experimental data were obtained using the Differential Scanning Calorimetry (DSC) technique for isobaric vapor-liquid equilibrium (VLE) of two binary mixtures at two different pressures (1.2 and 2.5 KPa): system 1 [monoacylglycerol (monocaprylin) + fatty acid (palmitic acid)] and system 2 [monoacylglycerol (monocaprylin) + fatty ester (methyl stearate)]. System 1 is relevant in the purification steps of the deodorizer distillates while system 2 is relevant in the purification steps of biodiesel and bioglycerol. A non-ideal behavior is revealed for both systems at the two different pressures, with azeotrope behavior observed and confirmed but the relative volatility analysis. Available thermodynamic consistency tests for TPx data were applied before performing parameter regressions for Wilson NRTL, UNIQUAC and original UNIFAC models. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC model. A new group for original UNIFAC model is created aiming to improve the representation of the experimental data.
by this predictive model.

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

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

**General information**
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**Ontology for pharmaceutical processes with focus on batch to continuous manufacturing**

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**Overview of CAPEC and ICAS**

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**Process intensification in integrated membrane processes**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technische Universität Dortmund
Authors: Lutze, P. (Ekstern), Gani, R. (Intern)
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Process synthesis, design and analysis using process-group contribution method
This paper describes the development and application of a framework for synthesis, design, and analysis of chemical and biochemical processes. The framework is based on the principle of group contribution used for prediction of physical properties. The fundamental pillars of this methodology are the definition and use of process-groups (building blocks) representing process operations, flowsheet connectivity rules to join the process-groups and flowsheet property models to evaluate the performance of the flowsheet structures. This framework for synthesis and design of chemical and biochemical processes along with the associated models and tools is generic and can be applied either to retrofit problems where improvement of an existing process flowsheet is desired or to design a new process flowsheet. Based on the framework, a prototype software has been developed and its application is highlighted through a case study involving the well-known HDA process. © 2014 Elsevier B.V.
Process Synthesis, Design and Analysis using Process-Group Contribution Method

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Kumar Tula, A. (Intern), Eden, M. R. (Intern), Gani, R. (Intern)
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Product Design – From Molecules to Formulations to Devices

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

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Hong Kong University of Science and Technology
Authors: Gani, R. (Intern), Ng, K. M. (Ekstern)
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Sustainable Process Networks for CO2 Conversion

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

General information

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Chulalongkorn University
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Sustainable Process Synthesis-Intensification

Sustainable process design can be achieved by performing process synthesis and process intensification together. This approach first defines a design target through a sustainability analysis and then finds design alternatives that match the target through process intensification. A systematic, multi-stage framework for process synthesis-intensification that identifies more sustainable process designs has been developed. At stages 1-2, the working scale is at the level of unit operations, where a base case design is identified and analyzed with respect to sustainability metrics. At stages 3-4, the working scales are at the levels of unit operations, tasks and phenomena. Here, first intensification flowsheet alternatives are generated through a task-based process synthesis method where tasks performed in unit operations are identified, analyzed and recombed through a means-ends analysis. Next, a phenomena-based process synthesis method is applied, where the phenomena involved in each tasks are identified, manipulated and recombed to generate new and/or existing unit operations configured into flowsheets that are more sustainable from those found in the previous levels. An overview of the key concepts and the framework are presented together with the results from a case study highlighting the
The chemical and biochemical industry needs major reductions in energy consumption, waste generation, number of equipment used in the construction of plants and capital/operational cost. These required reductions can be addressed through process intensification that is the efficient use of raw materials (feedstock) and the use of sustainable technologies.
or processes which directly impacts and improves sustainability/LCA factors. Process intensification is a concept by which processes, whether conceptual or existing, can be designed or redesigned to achieve more efficient and sustainable designs. Therefore sustainable process design can be achieved by performing process synthesis and process intensification together. The main contribution of this work is the development of a systematic computer-aided multi-scale, multi-level framework for performing process synthesis-intensification that aims to make a process more sustainable than a base case design, which represents either a new or existing process. The framework consists of eight steps (step 1 to step 8) that operates at the unit operation scale and task scale, and four integrated task-phenomena-based steps (IT-PBS.1 to IT-PBS.4) that operates at the task scale and phenomena scale. The concept of generating more sustainable designs through the combination of phenomena provides the opportunity to innovate through the generation of novel unit operations and thereby expand the search space of available unit operations. At the unit operations scale a conceptual base case design is synthesized through the sequencing of unit operations. The base case is then designed and analysed for identifying process limitations or bottlenecks (hot-spots) using a comprehensive analysis consisting of economic, life cycle and sustainability analyses that are translated into design targets. These hot-spots are associated with tasks that may be targeted for overall process improvement. Next an integrated task-phenomena-based synthesis method is applied, where the involved phenomena in various tasks are identified, manipulated and recombined using combination rules in order to generate new and/or existing unit operations that are configured into flowsheet alternatives inclusive of hybrid/intensified unit operations. The flowsheet alternatives that satisfy the performance criteria and design targets, give innovative and more sustainable, non-trade off flowsheet designs that otherwise could not be found from the higher scales. The framework is applied to three case studies related to the chemical and bioprocess industry in order to test the applicability of the framework for covering a wide range of applications, showing that process intensification provides major benefits related to the generation of more sustainable process designs.

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Sustainable Process Synthesis-Intensification

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Technical University of Dortmund
Authors: Babi, D. K. (Intern), Holtbruegge, J. (Ekstern), Lutze, P. (Ekstern), Górak, A. (Ekstern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2014
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Systematic computer aided framework for process synthesis, design and intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Gani, R. (Intern), Babi, D. K. (Intern)
Systematic Methodology for Design of Tailor-Made Blended Products: Fuels and Other Blended Products

A tailor-made blended liquid product is defined as a formulation of various chemicals in the liquid state to obtain a liquid mixture with a specific set of desired characteristics and qualities. Examples of blended liquid products are synthetic fuels and lubricants. This type of products is very important in daily life, since they not only keep people moving around, but also guarantee that machines and equipment work smoothly. The objective of this work is to tackle the blending problems using computer-aided tools for the initial stage of the product design.

A systematic methodology for design of tailor-made blended products has been developed, which has four main tasks. First, the design problem is defined: the product needs are identified, translated into target properties and the bounds for each target property are defined. Secondly, target property models are retrieved from a property model library. Thirdly, a mixture/blend design algorithm is applied to obtain the mixtures/blends that match the design targets. The result is a set of blends that match the constraints, the composition of the chemicals present in the blend, and the values of the target properties. Finally, the mixture target property values are verified by means of rigorous models for the properties and the mixtures. Besides the methodology, as the main contribution, specific supporting tools that were developed to perform each task are also important contributions of this research work.

The applicability of the developed methodology and tools was tested through two case studies. In the first case study, two different gasoline blend problems have been solved. In the second case study, four different lubricant design problems have been solved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. B. (Intern), Gani, R. (Intern), Gernaey, K. (Intern), Woodley, J. M. (Ekstern)
Number of pages: 173
Publication date: 2014

Publication information
Publisher: Technical University of Denmark, Department of Chemical and Biochemical Engineering
ISBN (Print): 978-87-93054-33-2
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Systematic_Methodology_for_Design.pdf
Publication: Research › Ph.D. thesis – Annual report year: 2014

Systematic Process Design and Operation of Intensified Processes

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

Nowadays, companies are looking for new sustainable design alternatives that improve their original processes. To assess the best design alternative, economic aspects have been the preferred indicators. However, environmental and social concerns should also be included in the decision process so that truly sustainable design alternatives can be found. This work proposes a framework, called ‘Techno-Economic Sustainability Environmental Impact Diagnosis’ (TESED) that allows users to assess chemical/biochemical processes in a product oriented analysis. TESED is a systematic and generic approach that can be applied to any product/processes combination. Bioethanol production was the case-study selected to highlight the TESED framework. Two production processes using two different feedstocks, hardwood chips and cassava rhizome, have been analysed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Universidade de Lisboa
Authors: Loureiro da Costa Lira Gargalo, C. (Intern), Carvalho, A. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern)
Number of pages: 6
Pages: 1021-1026
Publication date: 2014
Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.198 SNIP 0.215 CiteScore 0.48
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.245 SNIP 0.249 CiteScore 0.39
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.239 SNIP 0.217 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.216 SNIP 0.175 CiteScore 0.28
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.196 SNIP 0.267 CiteScore 0.33
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.194 SNIP 0.199 CiteScore 0.3
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.181 SNIP 0.135
Scopus rating (2009): SJR 0.16 SNIP 0.163
Scopus rating (2008): SJR 0.167 SNIP 0.124
Scopus rating (2007): SJR 0.182 SNIP 0.094
Scopus rating (2006): SJR 0.138 SNIP 0.108
Scopus rating (2005): SJR 0.178 SNIP 0.178
Scopus rating (2004): SJR 0.19 SNIP 0.161
Scopus rating (2003): SJR 0.157 SNIP 0.212
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.168 SNIP 0.214
Scopus rating (2001): SJR 0.146 SNIP 0.193
Scopus rating (2000): SJR 0.102 SNIP 0
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Original language: English
TESED, Bioethanol, Retrofit, Sustainability
The need and challenge to find more sustainable alternatives for the modern society

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

The Ontology System for Easy and Reusable Model Knowledge Representation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences

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

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Chulalongkorn University
Authors: Sueviriyapan, N. (Ekstern), Siemanond, K. (Ekstern), Quaglia, A. (Intern), Gani, R. (Intern), Suriyaphraphidalok, U. (Ekstern)
Pages: 133-138
Publication date: 2014
The Virtual Product-Process Design Lab

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

The Virtual Product-Process Design Laboratory for Structured Chemical Product Design and Analysis

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

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Kalakul, S. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Publication date: 2014
Main Research Area: Technical/natural sciences

**Bibliographical note**
ORAL PRESENTATION
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Achieving More Sustainable Solutions through Process Intensification

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Gani, R. (Intern), Babi, D. K. (Intern), Mansouri, S. S. (Intern), Ismail, M. I. (Ekstern), Huusom, J. K. (Intern), Woodley, J. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from 50th Anniversary Symposium of the Department of Chemical & Biological Engineering, Korea University, Seoul, Korea, Republic of.
Main Research Area: Technical/natural sciences

**Bibliographical note**
Oral presentation
Source: dtu
Source-ID: u::9372
Publication: Research › Conference abstract for conference – Annual report year: 2013

Achieving More Sustainable Solutions Through Process Intensification

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Gani, R. (Intern), Babi, D. K. (Intern), Mansouri, S. S. (Intern), Ismail, M. (Ekstern), Huusom, J. K. (Intern), Woodley, J. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9366
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Achieving sustainability through process intensification

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2013
Event: Abstract from SCPPE 2013, Dalian, China.
Main Research Area: Technical/natural sciences
**A Framework for Process Synthesis integrated with Sustainability and Process Intensification**

**General information**

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

**Bibliographical note**

Oral presentation

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

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

**General information**

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

**Publication information**

Journal: Chemical Engineering Research and Design
Volume: 91
Issue number: 10
ISSN (Print): 0263-8762
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- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.855 SNIP 1.449 CiteScore 2.7
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.957 SNIP 1.668 CiteScore 2.56
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
A Generic Life Cycle Assessment Tool for Chemical-biochemical Processes

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

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, DSM Chemtech Center
Authors: Hukkerikar, A. (Intern), Meier, R. J. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 23-32
Publication date: 2013
Main Research Area: Technical/natural sciences
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
Authors: Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9436
Publication: 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
Authors: Quaglia, A. (Intern), Gani, R. (Intern), Sin, G. (Intern), Sarup, B. (Ekstern)
Number of pages: 239
Publication date: 2013

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Publisher: Technical University of Denmark, Department of Chemical and Biochemical Engineering
ISBN (Print): 978-87-93054-08-0
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: 
Alberto Quaglia_PEC13-41.pdf

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

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

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Applications of Process Synthesis: Moving from Conventional Chemical Processes towards Biorefinery Processes

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from 9th World Congress of Chemical Engineering Incorporating 15th Asian Pacific Confederation of Chemical Engineering Congress, Seoul, Korea, Republic of.
Main Research Area: Technical/natural sciences

Bibliographical note
Invited Keynote oral presentation
Source: dtu
Source-ID: u::9369
Publication: Research › Conference abstract for conference – Annual report year: 2013

A Robust Process Analytical Technology (PAT) System Design for Crystallization Processes

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

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

A generic computer-aided framework for systematic design of a process monitoring and control system for crystallization processes has been developed to study various aspects of crystallization operations. The systematic design framework contains a generic crystallizer modelling toolbox, a tool for generation of the supersaturation set-point for supersaturation control, as well as a tool for design of a process monitoring and control system (also called Process Analytical Technology (PAT) system). This systematic design allows one to generate the necessary problem-chemical system specific model, the necessary supersaturation set-point as well as a PAT system design including implementation of monitoring tools and control strategies in order to produce the desired target product properties notably crystal size distribution (CSD) and shape for a wide range of crystallization processes. Application of the framework is highlighted through a case study involving the design of a monitoring and control system for a potassium dihydrogen phosphate (KDP) crystallization process, where also the one-dimensional CSD and two-dimensional CSD modelling features are highlighted.
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
Authors: Abdul Samad, N. A. F. B. (Intern), Meisler, K. T. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from BIWIC 2013, Odense, Denmark.
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::7430
Publication: 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 problem. Tools for the analysis of
the uncertainty, of its consequences on the decision-making process and for the identification of strategies to mitigate its
impact on network performances are integrated in the framework. A decomposition-based approach is employed to deal
with the added complexity of the optimization under uncertainty. A network benchmarking problem is proposed as a
benchmark for further development of methods, tools and solution approaches. To highlight the features of the framework,
a large industrial case study dealing with soybean processing is formulated and solved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa
Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 47-62
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 59
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.293 SNIP 2.127
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.625 SNIP 1.959
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.304 SNIP 1.936
Scopus rating (2005): SJR 1.314 SNIP 1.953
A Tool to Support Optimal Industrial Wastewater Treatment Design and Analysis

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
Authors: Quaglia, A. (Intern), Pennati, A. (Ekstern), Bozkurt, H. (Intern), Sin, G. (Intern), Gani, R. (Intern)
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Event:
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Industrial wastewater treatment, Water reuse and recycle, Refinery wastewater, Design and optimization
Source: dtu
Source-ID: u::9026
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Capec Consortium: Effective Academic-Industrial Interactions Strengthened By Surveys and Analyses of Gaps in Properties Modeling

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

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

General information
State: Published
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 model 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

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

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2013
Event: Poster session presented at 23rd European Symposium on Computer Aided Process Engineering, Lappeenranta, Finland.
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Source: dtu
Source-ID: u::8705
Publication: Research - peer-review › Poster – Annual report year: 2013

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
Authors: Fedorova, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 775-780
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Modeling framework, Fixed bed reactor, Computer-aided modeling.
Source: dtu
Source-ID: u::8705
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013
Computer aided solvent selection, design and application

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Number of pages: 1
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Event: Abstract from Bayer lecture, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Center for Process Engineering and Technology
Authors: Meisler, K. T. (Intern), von Solms, N. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Pages: 176-183
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Main Research Area: Technical/natural sciences
Conference: BIWIC 2013, Odense, Denmark, 18/09/2013 - 18/09/2013
Source: dtu
Source-ID: u::9395
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, State University of Campanas, Alfa Laval Copenhagen A/S, University of Virginia
Authors: Cunico, L. (Intern), Ceriani, R. (Ekstern), Sarup, B. (Ekstern), O’Connell, J. P. (Ekstern), Gani, R. (Intern)
Pages: 318–327
Publication date: 2013
Main Research Area: Technical/natural sciences
Data, analysis, modeling, and prediction of properties and phase equilibria for process design of edible oil and biodiesel systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S, University of Virginia, State University of Campinas
Authors: Cunico, L. (Intern), Ceriani, R. (Ekstern), Sarup, B. (Ekstern), O’Connell, J. P. (Ekstern), Gani, R. (Intern)
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Publication date: 2013
Event: Poster session presented at PPEPPD 2013, Puerto Iguazu, Argentina.
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Denmark's Chemicals Industry: Progress and Challenges

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

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BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.165 SNIP 0.188 CiteScore 0.33
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.218 SNIP 0.353 CiteScore 0.29
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.32 SNIP 0.687 CiteScore 0.39
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.425 SNIP 0.665 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.539 SNIP 0.732 CiteScore 0.64
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.63 SNIP 0.947 CiteScore 0.41
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Design methodology for bio-based processing: Biodiesel and fatty alcohol production

A systematic design methodology is developed for producing multiple main products plus side products starting with one or more bio-based renewable source. A superstructure that includes all possible reaction and separation operations is generated through thermodynamic insights and available data. The number of alternative processes is systematically reduced through a screening procedure until only feasible alternatives are obtained. As part of the methodology, process intensification involving reaction–separation tasks is also considered to improve the design by shifting the equilibrium reactions. Economic analysis and net present value are determined to find the best economically and operationally feasible process. The application of the methodology is presented through a case study involving biodiesel and fatty alcohol productions.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Chulalongkorn University
Authors: Simasatikul, L. (Ekstern), Arpornwichanopa, A. (Ekstern), Gani, R. (Intern)
Pages: 48-62
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 57
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 661-666
Publication date: 2013
Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Columbia University
Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Pages: 817-822
Publication date: 2013

Design of sustainable blended products using an integrated methodology

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Columbia University
Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Publication date: 2013
Event: Poster session presented at 23rd European Symposium on Computer Aided Process Engineering, Lappeenranta, Finland.
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9032
Publication: Research - peer-review › Poster – Annual report year: 2013
Design of Sustainable Blended Products using an Integrated Methodology

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

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

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

Commercial and industrial detergents, formulated liquid blends, have recently become extremely sophisticated, in order to address a broad range of cleaning tasks and to deliver superior performances with a minimum of effort and time. These products, by definition, consist of different chemicals, each with a specific function related to the needs of the product: surfactants, builders, bleaching agents, enzymes and minors, usually mixed together with a carrier, necessary to keep the blend as a homogeneous liquid formulation. A system approach and associated tools can help to virtually generate and test different candidates in order to identify the most promising formulations before a detailed experimental stage for final selection and product development is applied. In this way, the whole design
prediction of properties is important in chemical process-product design. Reliable property models are needed for increasingly complex and wider range of chemicals. Group-contribution methods provide useful tool but there is a need to validate them and improve their accuracy when complex chemicals are present in the mixtures. In accordance with that, a combined group-contribution and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties. This so-called Group- ContributionPlus (GCPlus) approach is a hybrid model which combines group contribution and molecular descriptor theories (such as connectivity indices – CI). Connectivity indices are formalisms defined via graph theoretical concepts intended to describe the topological characteristics of molecular structures. The main idea is the use of connectivity indices to describe the molecular fragmentation that relates properties which is the molecular interactions with the molecular structures. One well known and established group-contribution method is the UNIFAC model, used to predict liquid phase activity coefficients for mixtures. The needed values of the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are, however many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, which may not be feasible, values of the missing GIPs, can be predicted through the GCPlus approach. The predicted values for the GIPs are then used in the UNIFAC model to calculate activity coefficients. This approach can increase the application range of any “host” UNIFAC model by providing a reliable predictive model towards fast and efficient product development.
This PhD project is focused on the analysis and further development of the GCPlus approach for predicting mixture properties to be called the UNIFAC-CI model. The contributions of this work include an analysis of the developed Original UNIFAC-CI model in order to investigate why the model does not perform as well as the reference UNIFAC model for some systems while performing surprisingly better than the reference model for other systems. In this analysis, it is found that by introducing more structural information to the CHO group through the valence connectivity index (CI), the correlation error involving alkanes-aldehydes system can be reduced. This work is presented in Chapter 3. Furthermore in Chapter 4, as a continuation of the analysis done for systems involving C, H and O atoms, the Original UNIFAC-CI (VLE) model has been further reused and significantly expanded by including nitrogenated, chlorinated and sulfated systems and the involved atom interaction parameters (AIPs) have been regressed. In addition to that, another set of parameters have been generated for the Original UNIFAC-CI (VLE) model using a quality assessment algorithm, QVLE (combination of 4 VLE consistency tests) as a weighting factor for each VLE dataset in the objective function for regression of AIPs. The quality factors are useful in identifying anomalous systems which can be problematic in the parameter estimation and can produce parameters which are not accurately representing the systems used for the regression. Moreover, in Chapter 5 the Original UNIFAC-CI (VLE/SLE) model has been developed where the atom interaction parameters (AIPs) are obtained through regression against both VLE and SLE experimental data. The prediction accuracy of SLE systems using the regressed parameters has been slightly increased. Besides that, in Chapter 6, Modified (Dortmund) UNIFAC-CI has been further developed by including chlorinated and sulfated VLE systems. Finally, in Chapter 7, the developed Original UNIFAC-CI (VLE/SLE) model has been highlighted in selected case studies involving the design of a working solution for hydrogen peroxide production and solubility investigation of pharmaceutical systems where new group have been created and their interaction parameters are predicted/fine tuned generating a master parameter table specifically for those case studies. Also, the applicability of the Original UNIFACCI model is shown for predicting phase equilibria of lipid systems, filling missing GIPs and improving prediction of azeotropic mixture. In Chapter 8, a discussion with concluding remarks and recommendation for future work are presented.
an 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.
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.293 SNIP 2.127
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.625 SNIP 1.959
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.304 SNIP 1.936
Scopus rating (2005): SJR 1.314 SNIP 1.953
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.125 SNIP 1.908
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.348 SNIP 1.936
Scopus rating (2002): SJR 1.042 SNIP 0.92
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.955 SNIP 0.728
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.366 SNIP 1.025
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.073 SNIP 1.113
Original language: English
DOIs:
10.1016/j.compchemeng.2012.11.003
Source: dtu
Source-ID: n:oai:DTIC-ART:elsevier/375012157::22239
Publication: Research › Editorial – Annual report year: 2013
Main features of SustainPro are illustrated through a case study of ß-Galactosidase production. The application and the end the design alternatives, are evaluated using environmental impact assessment tools and safety indices. The extended SustainPro guides the user through the necessary steps according to work-flow of the implemented methodology. At the process information/data such as the process flowsheet, the associated mass / energy balance data and the cost data, extended systematic methodology for sustainable process design (Carvalho et al. 2008 and Carvalho et al. 2009). Using chemical processes operating in batch or continuous modes. The software tool is based on the implementation of an environment and social issues. This paper presents the development of a software tool (SustainPro) and its application to Chemical processes are continuously facing challenges from the demands of the global market related to economics, wastewater treatment and reuse; municipal water treatment) and biorefinery.

Activities:
Efficient Information and Data Management in Synthesis and Design of Processing Networks
SustainPro - A tool for systematic process analysis, generation and evaluation of sustainable design alternatives
Efficient Information and Data Management in Synthesis and Design of Processing Networks
SustainPro - A tool for systematic process analysis, generation and evaluation of sustainable design alternatives

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2013
Main Research Area: Technical/natural sciences

Relations
Activities:
Efficient Information and Data Management in Synthesis and Design of Processing Networks
Efficient Information and Data Management in Synthesis and Design of Processing Networks
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.
Generic Modelling Framework for Design and Analysis of Crystallization Operations

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Meisler, K. T. (Intern), Abdul Samad, N. A. F. B. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
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Industry-academia collaboration through the CAPEC industrial consortium

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from Pfizer seminar, Hartford, CT, United States.
Main Research Area: Technical/natural sciences

Bibliographical note
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from 9th World Congress of Chemical Engineering Incorporating 15th Asian Pacific Confederation of Chemical Engineering Congress, Seoul, Korea, Republic of.
Main Research Area: Technical/natural sciences

Bibliographical note
Invited keynote oral presentation
Publication: Research › Conference abstract for conference – Annual report year: 2013

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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Abdul Samad, N. A. F. B. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
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Managing the Complexity in Chemical Product Engineering

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
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Main Research Area: Technical/natural sciences

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Model-Based Blend Design: Application to Lubricant Oils

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. B. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
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Main Research Area: Technical/natural sciences
Lubricant, Base oil, Model-based approach, Product design
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Model based methods and tools for process systems engineering

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

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
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Source: dtu
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Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group-Contribution Method

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel

The knowledge of physical and thermodynamic properties of pure components and their mixtures is a basic requirement for performing tasks related to process design, simulation, and optimization and also for performing chemical product design using computer aided molecular/mixture design (CAMD) tools. With an increasing trend in the production rates of edible oils, fats and other lipids, accurate prediction of the necessary properties (pure component and mixture) has become a major concern and issue. The mixtures handled consist of large complex chemicals such as fatty esters, acids, alcohols, glycerides, sterols, etc., with or without the presence of water. Because of the lack of measured data, it is necessary to have available truly predictive but reliable models requiring very little data for their development. A systematic numerical analysis to identify the needs of phase equilibria and related properties in process design and analysis for the production of edible oils and related products has been done and from this analysis the requirements of a database with respect to model development has been established. In total, 333 different phase equilibrium systems (91 VLE, 91 LLE, 70 SLE), 80 solubility systems, and around 4500 data points on phase equilibria has been found in addition to 8 pure component properties for 290 lipids. The consistency of the available VLE data has been checked with six tests (Van Ness, Herington or Area, Point or Differential, Infinite Dilution, Pure component and EOS), using a general and robust approach developed by Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST). It was found that most of the data failed, at least one of these tests. Nevertheless, using data-quality factors, all data have been used to regress parameters of UNIFAC model. This procedure has also been repeated for SLE-data, where new thermodynamic consistency tests are proposed. The performance of molecular models (UNIQUAC, UNIFAC, and NRTL) as well as GC+ approach based UNIFAC-CI method is discussed and compared for phase equilibria calculations. For lipids systems, a special set of group-interaction parameters have been determined to make the GC-based models more predictive. These results are then used to obtain interaction parameters for the PC-SAFT to add further predictive power.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
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Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences

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Activities:
Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel
Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel
Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel

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

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

General information
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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.

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

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
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Number of pages: 1
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Event: Poster session presented at PPEPPD 2013, Puerto Iguazu, Argentina.
Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Poster – Annual report year: 2013
Optimal Design of Microalgal Biomass Processing Network

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Korea Advanced Institute of Science & Technology
Authors: Lee, J. H. (Ekstern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u:9432
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Optimal processing pathway for the production of biodiesel from microalgal biomass: A superstructure based approach
In this study, we propose a mixed integer nonlinear programming (MINLP) model for superstructure based optimization of biodiesel production from microalgal biomass. The proposed superstructure includes a number of major processing steps for the production of biodiesel from microalgal biomass, such as the harvesting of microalgal biomass, pretreatments including drying and cell disruption of harvested biomass, lipid extraction, transesterification, and post-transesterification purification. The proposed model is used to find the optimal processing pathway among the large number of potential pathways that exist for the production of biodiesel from microalgae. The proposed methodology is tested by implementing on a specific case with different choices of objective functions. The MINLP model is implemented and solved in GAMS using a database built in Excel. The results from the optimization are analyzed and their significances are discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Korea Advanced Institute of Science & Technology
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
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Phenomena based Methodology for Process Synthesis incorporating Process Intensification

Process intensification (PI) has the potential to improve existing as well as conceptual processes, in order to achieve a more sustainable production. PI can be achieved at different levels. That is, the unit operations, functional and/or phenomena level. The highest impact is expected by looking at processes at the lowest level of aggregation which is the phenomena level. In this paper, a phenomena based synthesis/design methodology incorporating process intensification is presented. Using this methodology, a systematic identification of necessary and desirable (integrated) phenomena as well as generation and screening of phenomena based flowsheet options are presented using a decomposition based solution approach. The developed methodology as well as necessary tools and supporting methods are highlighted through a case study involving the production of isopropyl-acetate.

General information
State: Published
Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
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Web of Science (2016): Indexed yes
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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
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Web of Science (2013): Indexed yes
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ISI indexed (2012): ISI indexed yes
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BFI (2010): BFI-level 2
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Web of Science (2005): Indexed yes
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Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
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DOIs:
Predicting Surfactant-related Properties for Chemical-based Product Design

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences

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

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Conte, E. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 36
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Publisher: Wiley-VCH
Editors: Broeckel, V., Wagner, D., Meier, W.
Main Research Area: Technical/natural sciences
DOIs: 10.1002/9783527654741.ch5
Source: dtu
Source-ID: u::9557
Publication: Research - peer-review › Book chapter – Annual report year: 2013

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Universidad Estadual de Campinas, Virginia Polytechnic Institute and State University
Authors: Ceriani, R. (Ekstern), Gani, R. (Intern), Liu, Y. (Ekstern)
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.
Selection and design of solvents

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

Software Integration of Life Cycle Assessment and Economic Analysis for Process Evaluation

This study is focused on the sustainable process design of bioethanol production from cassava rhizome. The study includes: process simulation, sustainability analysis, economic evaluation and life cycle assessment (LCA). A steady state process simulation if performed to generate a base case design of the bioethanol conversion process using cassava rhizome as a feedstock. The sustainability analysis is performed to analyze the relevant indicators in sustainability metrics, to definedesign/retrofit targets for process improvements. Economic analysis is performed to evaluate the profitability of the process. Also, simultaneously with sustainability analysis, the life cycle impact on environment associated with bioethanol production is performed. Finally, candidate alternative designs are generated and compared with the base case design in terms of LCA, economics, waste, energy usage and environmental impact in order to identify the most sustainable design for the production of ethanol. The capacity for ethanol production from cassava rhizome is set to 150,000 liters/day, which is about 1.3 % of the total demand of ethanol in Thailand. LCA on the base case design pointed to large amounts of CO2 and CO emissions (related to combustion engine from transportation), biowaste and waste water that are released from the distillation columns, which affect the terrestrial ecotoxicity. Sustainability analysis on the base case pointed to a large waste of the water and lignin, which were then targeted for potential improvement.
Study of Crystallization Kinetics Within a Generic Modelling Framework

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Loughborough University
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Superstructure optimization of biodiesel production from microalgal biomass

In this study, we propose a mixed integer nonlinear programming (MINLP) model for superstructure based optimization of biodiesel production from microalgal biomass. The proposed superstructure includes a number of major processing steps for the production of biodiesel from microalgal biomass, such as harvesting of microalgal biomass, pretreatments including drying and cell disruption of harvested biomass, lipid extraction, transesterification, and post-transesterification purification. The proposed model is used to find the optimal processing pathway among the large number of potential pathways that exist for the production of biodiesel from microalgae. The proposed methodology is tested by implementing on a specific case study. The MINLP model is implemented and solved in GAMS using a database built in Excel. The results from the optimization are analyzed and their significances are discussed.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Korea Advanced Institute of Science & Technology
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Biodiesel, Microalgae, Superstructure optimization, Mixed integer nonlinear programming, Biorefinery
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Sustainable and Intensified Design of a Biodiesel Production Process
The growing concerns about the global warming and greenhouse gas emissions (GHG) have led to an increase in the interest to produce fuel from biomass and from the fact that such fuels can relieve the reliance on imported oil and price. To this end, numerous production facilities are being set up, at different scales and using different methods of manufacture based on different raw materials and component properties [1]. It is therefore timely to study the sustainability and feasibility of these various manufacturing routes. Therefore, finding the best alternative and design with minimum environmental impact and maximum profitability is needed. In this work a computer-aided framework for process synthesis and process intensification is applied for sustainable production of biodiesel from pure/waste palm oil as the feedstock. This approach examines several biodiesel processing routes that were collected through available data and current technologies reported in the literature. Using this information, a generic superstructure of processing routes was created that described a network of configurations representing multiple designs for the production of biodiesel. Therefore, based on the currently known technologies, this superstructure includes all possible alternatives. The next step was to analyze the superstructure in terms of economic and sustainability metrics. This was done by first performing simulation to obtain the steady state mass and energy balance data for the entire superstructure. These data were then used for a sustainability analysis [2] where a set of calculated closed- and open-path indicators were employed to identify the structural bottlenecks within the superstructure. Based on this analysis the number of process alternatives within the superstructure was reduced and a set of feasible flowsheet alternatives were identified. These were further reduced through economic and lifecycle assessment analysis (LCA) to determine the alternative that best matched a specified set of performance criteria (or design targets). A rigorous simulation was performed on this flowsheet, which at this stage was considered as the base case design for the next step of the framework. To further improve the base case design, process intensification was considered [3] with the targets set by LCA, economic and sustainability analyses in the previous step. Out of the three available levels for achieving PI, the phenomena-level, which is the lowest level of aggregation, was considered so that potentially new and improved alternatives to the base case design could be obtained. The objective (or target) for the intensified process design was to overcome the bottlenecks of the base case design. The optimization problem was further refined in terms of logical, operational, structural constraints, using a PI knowledge base tool. The next step was to identify the phenomena representing the tasks performed within the base case design and the operating window of each phenomenon, by applying thermodynamic insights [4] and the PI knowledge base. Next, the phenomena needed to overcome all identified process bottlenecks were identified, sorted in terms of operation (task) types and the phenomena present in them, and, screened using structural, operational and thermodynamic information. Note that different combinations of phenomena can perform the same specified task. The phenomena were then combined according to a set of rules to form unit operations, which in turn were combined to form new and innovative process alternatives. Finally, from the remaining set of feasible intensified process alternatives, the best in terms of economic and environmental sustainability was identified. For the case of biodiesel production, the intensified process alternative turned out to be the most economical and more sustainable than other alternatives. The computer-aided methods and tools used in this work are: SustainPro (method and tool for process sustainability analysis), ECON (method and tool for process economic analysis), LCSoft (method and tool for process lifecycle assessment analysis) and process simulation software (e.g. PRO/II, ASPEN Plus, ICAS). They are all used in an integrated framework for process synthesis.

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Organisations: Department of Energy Conversion and Storage, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
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Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013
**Sustainable Intensified Process Retrofit for the Production of MDI**

Process intensification (PI) is a means by which processes can be made more efficient and sustainable at different levels, the unit operations, functional and phenomena levels. Therefore PI can be used for making process improvements at the functional level for the production of an important polyurethane, methylene diphenyl-di-isocyanate (MDI).

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Huntsman Polyurethanes Limited
Authors: Babi, D. K. (Intern), Woodley, J. (Intern), Gani, R. (Intern), Jones, D. (Ekstern), Zeeuw, A. J. (Ekstern)
Number of pages: 1
Publication date: 2013

**Sustainable Process Design of Bioethanol Production from Cassava rhizome**

This study is focused on the sustainable process design of bioethanol production from cassava rhizome. The study includes: process simulation, sustainability analysis, economic evaluation and life cycle assessment (LCA). A steady state process simulation is performed to generate a base case design of the bioethanol conversion process using cassava rhizome as a feedstock. The sustainability analysis is performed to analyze the relevant indicators in sustainability metrics, to defined retrofit targets for process improvements. Economic analysis is performed to evaluate the profitability of the process. Also, simultaneously with sustainability analysis, the life cycle impact on environment associated with bioethanol production is performed. Finally, candidate alternative designs are generated and compared with the base case design in terms of LCA, economics, waste, energy usage and environmental impact in order to identify the most sustainable design for the production of ethanol. The capacity for ethanol production from cassava rhizome is set to 150,000 liters/day, which is about 1.3% of the total demand of ethanol in Thailand. LCA on the base case design pointed to large amounts of CO2 and CO emissions (related to combustion engine from transportation), biowaste and waste water that are released from the distillation columns, which affect the terrestrial ecotoxicity. Sustainability analysis on the base case pointed to a large waste of the water and lignin, which were then targeted for potential improvement.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Chulalongkorn University
Authors: Mangnimit, S. (Ekstern), Malakul, P. (Ekstern), Gani, R. (Intern)
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**Host publication information**

Title of host publication: Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA)
Main Research Area: Technical/natural sciences
Sustainable, Process design, Bioethanol, Cassava rhizome

**Sustainable Process Design of Lignocellulose based Biofuel**

Worldwide energy demand has increased steadily as the world population has grown and more countries have become industrialized. The major energy sources of the world still depend on fossil fuels, which are also the main sources for carbon dioxide emission. As the fossil fuels always pass through a combustion processing step, carbon dioxide and other important greenhouse gases are released. This is considered non-renewable and non-sustainable energy and may be one
of the major causes of global warming and therefore, climate change concerns coupled with high oil prices. This is driving efforts to increase the production and use of alternative and sustainable energy sources as rapidly as possible. Biofuel is a type of alternative energy that can be produced from many sources including sugar substances (such as sugarcane juice and molasses), starchy materials (such as corn and cassava), and lignocellulosic materials such as agricultural residual, straw and wood chips, the residual from wood industry. However, those sugar and starchy materials can be used not only to make biofuels but they are also food sources. Thus, lignocellulosic materials are interesting feed-stocks as they are inexpensive, abundantly available, and are also non-food crops. In this respect, Cassava rhizome has several characteristics that make it a potential feedstock for fuel ethanol production. It has high content of cellulose and hemicelluloses.

The objective of this paper is to present a study focused on the sustainable process design of bioethanol production from cassava rhizome using various computer aided tools through a systematic and efficient work-flow. The study includes process simulation, sustainability analysis, economic evaluation and life cycle assessment (LCA) according to a well-defined workflow that guarantees the determination of sustainable process options, if they exist. The paper will highlight an improved alternative process design compared to a base case (published) design in terms of production cost, waste, energy usage and environmental impacts, criteria that are associated with sustainable process design. The final process design includes 39 unit operations, has a capacity of 150,000 L/day and produces dry ethanol (approximately 13.0% of cassava rhizome is converted to ethanol).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Chulalongkorn University
Authors: Mangnimit, S. (Ekstern), Malakul, P. (Ekstern), Gani, R. (Intern)
Number of pages: 1
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Event: Abstract from 9th World Congress of Chemical Engineering Incorporating 15th Asian Pacific Confederation of Chemical Engineering Congress, Seoul, Korea, Republic of.
Main Research Area: Technical/natural sciences
Sustainable, Process design, Bioethanol, Lignocellulosic materials, Life cycle assessment

Bibliographical note
Oral conference presentation.
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Systematic Design of Tailor-Made Blended Products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. B. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Number of pages: 1
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Systematic Design of Tailor-Made Blended Products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences
Product design, Computer-aided approach, Gasoline, Lubricant
Source: dtu
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Systematic Design of Tailor-Made Blended Products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. B. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9108
Publication: Research - peer-review › Poster – Annual report year: 2013

Systematic substrate adoption methodology (SAM) for future flexible, generic pharmaceutical production processes
The discovery of an effective and safe pharmaceutical product is based on success in clinical trials. Often, several candidate compounds targeting the same disease area are tested in order to identify the most efficacious products. This involves the manufacture of small quantities of compounds (APIs) for early delivery campaigns. Of these candidates only a few will be successful such that further development is required to scale-up the process. Systematic computer-aided methods and tools are required for faster manufacturing of these API candidates. In this work, a substrate adoption methodology (SAM) for a series of substrates with similar molecular functionality has been developed. The objective is to achieve "flexible, fast and future" pharmaceutical production processes by adapting a generic modular process template. Application of the methodology is illustrated through a case study from the pharmaceutical industry. Use of computer-aided methods and tools as part of the methodology is also highlighted.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center, AstraZeneca
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Main Research Area: Technical/natural sciences

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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Systematic sustainable process design and analysis of biodiesel processes

Biodiesel is a promising fuel alternative compared to traditional diesel obtained from conventional sources such as fossil fuel. Many flowsheet alternatives exist for the production of biodiesel and therefore it is necessary to evaluate these alternatives using defined criteria and also from process intensification opportunities. This work focuses on three main aspects that have been incorporated into a systematic computer-aided framework for sustainable process design. First, the creation of a generic superstructure, which consists of all possible process alternatives based on available technology. Second, the evaluation of this superstructure for systematic screening to obtain an appropriate base case design. This is done by first reducing the search space using a sustainability analysis, which provides key indicators for process bottlenecks of different flowsheet configurations and then by further reducing the search space by using economic evaluation and life cycle assessment. Third, the determination of sustainable design with/without process intensification using a phenomena-based synthesis/design method. A detailed step by step application of the framework is highlighted through a biodiesel production case study.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
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Pages: 167-202
Publication date: 2013

ThermoData Engine (TDE) is the first full-scale software implementation of the dynamic data evaluation concept, as reported in this journal. The present paper describes the first application of this concept to the evaluation of thermophysical properties for material streams involving any number of chemical components with assessment of uncertainties. The method involves construction of Redlich-Kister type equations for individual properties (excess volume, thermal conductivity, viscosity, surface tension, and excess enthalpy) and activity-coefficient models for phase equilibrium properties (vapor-liquid equilibrium). Multi-component models are based on those for the pure-components and all binary subsystems evaluated on demand through the TDE software algorithms. Models are described in detail, and extensions to the class structure of the program are provided. Novel program features, such as ready identification of key measurements for subsystems that can reduce the combined uncertainty for a particular stream property, are described. In addition, new product-design features are described for selection of solvents for optimized crystal dissolution, separation of binary crystal mixtures, and solute extraction from a single-component solvent. Planned future developments are summarized.

General information

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, National Institute of Standards and Technology, Korea University
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BFI (2016): BFI-level 1
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.582 SNIP 1.3 CiteScore 4.27
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.447 SNIP 1.259 CiteScore 3.88
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.647 SNIP 1.345 CiteScore 4.4
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.506 SNIP 1.354 CiteScore 4.22
Uncertainty and Sensitivity Analysis on PAT System Performance for Crystallization Processes

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Abdul Samad, N. A. F. B. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2013
Main Research Area: Technical/natural sciences
Crystallization, PAT system, Uncertainty analysis, Sensitivity analysis

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Use of Water-Oil-Surfactant System Phase Behavior Data/Model for Emulsion-based Chemical Product Design

Electronic versions:
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DOIs:
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A systematic synthesis and design methodology to achieve process intensification in (bio)chemical processes

Process intensification (PI) has the potential to improve existing processes or create new process options, which are needed in order to produce products using more sustainable methods. In principle, an enormous number of process options can be generated but where and how the process should be intensified for the biggest improvement is difficult to identify. In this paper the development of a systematic computer aided model-based synthesis and design methodology incorporating PI is presented. In order to manage the complexities involved, the methodology employs a decomposition-based solution approach. Starting from an analysis of existing processes, the methodology generates a set of process options and reduces their number through several screening steps until from the remaining options, the optimal is found. The application of the methodology is highlighted through a case study involving the chemo-enzymatic synthesis of N-acetyl-d-neuraminic acid (Neu5Ac).
Acceleration of pharmaceutical production by using micro-reactor technology in a continuous mode

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, CHEC Research Centre, Computer Aided Process Engineering Center, H. Lundbeck A/S
Number of pages: 2
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
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Source-ID: u::4323
Publication: Research - peer-review › Paper – Annual report year: 2012

Achieving process intensification form the application of a phenomena based synthesis, Design and intensification methodology
Process Intensification/Process Systems Engineering.

Process intensification (PI) is a means by which one can achieve a more efficient and sustainable chemical process. Major
success in the area of PI has been achieved by Eastman chemicals [1] which in 1984 intensified the process for the manufacture of methyl acetate by replacing with one single reactive distillation column the multi-step process which consisted of one reactor, extractive distillation, liquid-liquid separation and azeotropic distillation. However, except for reactive distillation and dividing wall columns, the implementation of PI still faces challenges [2] because the identification and design of intensified processes is not simple [3]. Lutze et al [3] has developed a systematic PI synthesis/design method at the unit operations (Unit-Ops) level, where the search space is based on a knowledge-base of existing PI equipment. Siirola [4] has proposed a task-based approach known as the means-ends analysis. A limitation with the means-ends analysis is that it becomes difficult to apply if too many corrective tasks should be identified and replaced and if too many alternatives should be considered. From the above PI methods, the starting point is knowledge of existing Unit-Ops and therefore a limitation arising from their application is that they are able to generate new integrations/combinations of intensified equipment but are unable to generate novel PI solutions employing new Unit-Ops. Therefore, incentives exist for a more systematic, efficient and flexible PI methodology covering a wider range of applications which is able to find truly innovative and predictive solutions, not only using knowledge of the existing methods at the Unit-Ops level but also operating at a lower level of aggregation (that is, the phenomena level). This enables the use of apriori knowledge of the Unit-Ops as well as the possibility to design new Unit-Ops. A first version for a phenomena-based synthesis/design (PhenPI) methodology has been developed [5] in which a process flowsheet is generated through the use of involved phenomena such as mixing, phase transition and phase separation [5]. In principle, generating processes from phenomena leads to a large number of process options and therefore, an efficient solution procedure for the evaluation of these process options is needed. To manage this complexity, the PhenPI methodology uses a decomposition based solution approach which breaks down the complex mathematical synthesis/design problem into manageable subproblems (6 steps). It allows the generation of PI options and their subsequent stepwise reduction of the search space and identification of the best intensified process option. In step-1, the problem definition of the process to be intensified. In step-2, the process is analyzed based on the base case design and the flowsheet is converted into a task and phenomena based flowsheet. In step-3, analysis of the process at the task and phenomena level and the use of different tools such as analysis of pure component and mixture properties are used to identify limitations/bottlenecks of the process. From this data, desirable tasks and suitable phenomena are identified to overcome these limitations/bottlenecks and for the processing of tasks in the most efficient manner. In step-4, the involved phenomena are aggregated and/or connected using a set of connectivity rules based on the operating windows of each phenomenon. Based on this, a large number of flowsheet options are generated which are subsequently screened for feasibility by applying logical and structural constraints. In step-5, the remaining flowsheet options are fast screened by constraints for feasibility and for performance using a set of PI performance metrics. The most promising phenomena-based options are transformed into a unit-operation based flowsheet using a set of rules. In step-6, the most promising unit-operation based options from step-5 are optimized in order to identify the best process option. In this paper the PhenPI methodology is presented in detail and highlighted by its application to the production of methyl acetate in order to identify the best PI option with respect to sustainability and other processes requiring reaction-separation processing tasks. It will be shown that the PhenPI methodology systematically not only generates the reactive distillation option proposed by Siirola but also other alternatives which have not been previously considered.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Babi, D. K. (Intern), Lutze, P. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from ANQUE ICCE 2012, Sevilla, Spain.
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation.

References:

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Publication: Research › Conference abstract for conference – Annual report year: 2012
Active pharmaceutical ingredient (API) production involving continuous processes – A process system engineering (PSE)-assisted design framework

A systematic framework is proposed for the design of continuous pharmaceutical manufacturing processes. Specifically, the design framework focuses on organic chemistry based, active pharmaceutical ingredient (API) synthetic processes, but could potentially be extended to biocatalytic and fermentation-based products. The method exploits the synergic combination of continuous flow technologies (e.g., microfluidic techniques) and process systems engineering (PSE) methods and tools for faster process design and increased process understanding throughout the whole drug product and process development cycle. The design framework structures the many different and challenging design problems (e.g., solvent selection, reactor design, and design of separation and purification operations), driving the user from the initial drug discovery steps – where process knowledge is very limited – toward the detailed design and analysis. Examples from the literature of PSE methods and tools applied to pharmaceutical process design and novel pharmaceutical production technologies are provided along the text, assisting in the accumulation and interpretation of process knowledge. Different criteria are suggested for the selection of batch and continuous processes so that the whole design results in low capital and operational costs as well as low environmental footprint. The design framework has been applied to the retrofit of an existing batch-wise process used by H. Lundbeck A/S to produce an API: zuclopenthixol. Some of its batch operations were successfully converted into continuous mode, obtaining higher yields that allowed a significant simplification of the whole process. The material and environmental footprint of the process – evaluated through the process mass intensity index, that is, kg of material used per kg of product – was reduced to half of its initial value, with potential for further reduction. The case-study includes reaction steps typically used by the pharmaceutical industry featuring different characteristic reaction times, as well as L–L separation and distillation-based solvent exchange steps, and thus constitutes a good example of how the design framework can be useful to efficiently design novel or already existing API manufacturing processes taking advantage of continuous processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, CHEC Research Centre, Computer Aided Process Engineering Center, H. Lundbeck A/S
Authors: Cervera Padrell, A. E. (Intern), Skovby, T. (Ekstern), Kiil, S. (Intern), Gani, R. (Intern), Gernaey, K. (Intern), Lutze, P. (Intern)
Pages: 437-456
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.49 SJR 1.366 SNIP 1.409
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.414 SNIP 1.496 CiteScore 4.37
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.469 SNIP 1.586 CiteScore 4.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.558 SNIP 1.706 CiteScore 4.64
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.976 SNIP 1.933 CiteScore 5.15
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 1.794 SNIP 1.887 CiteScore 4.77
ISI indexed (2011): ISI indexed yes
Adaptive Continuous Template-Based Novel Manufacturing Technique for Faster Manufacturing of New APIs for Clinical Trials

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences

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Links:
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Bibliographical note
Oral presentation.
Source: dtu
Source-ID: u::5321
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

A framework for the design of reacting systems with phase transfer catalysis
A generic modelling framework for phase transition catalyst based reacting systems has been developed and converted into a software tool. The modelling framework accommodates models of different types representing different sub-systems of the PTC-based reactive system; databases of model parameters and carefully collected and checked (for thermodynamic consistency) experimentally measured data. The models, data and software have been tested on various PTC-based reactive systems. Illustrative examples are provided.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Jealott's Hill International Research Center, University of Virginia
Authors: Piccolo, C. (Intern), Shaw, A. (Ekstern), Hodges, G. (Ekstern), Piccione, P. M. (Ekstern), O'Connell, J. P. (Ekstern), Gani, R. (Intern)
A framework for the design of reacting systems with phase transfer catalysis

A generic modelling framework for phase transition catalyst based reacting systems has been developed and converted into a software tool. The modelling framework accommodates models of different types representing different sub-systems of the PTC-based reactive system; databases of model parameters and carefully collected and checked (for thermodynamic consistency) experimentally measured data. The models, data and software have been tested on various PTC-based reactive systems. Illustrative examples are provided.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Jealott's Hill International Research Center, University of Virginia
Authors: Piccolo, C. (Intern), Shaw, A. (Ekstern), Hodges, G. (Ekstern), Piccione, P. M. (Ekstern), O'Connell, J. P. (Ekstern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Phase transfer catalysis, Modelling, Partition coefficient, Solubility, Design/analysis

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Poster presentation
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Source-ID: u::4475
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A generic framework for systematic design of a process monitoring and control system for crystallization processes has been developed in order to obtain the desired end-product properties notably the crystal size distribution (CSD). The design framework contains a generic crystallizer modelling tool-box, a tool for design of operational policies as well as a tool for design of process monitoring and control systems. Through this framework, it is possible for a wide range of crystallization processes to generate the necessary problem-system specific model, the necessary operational policy and a Process Analytical Technology (PAT) system design including implementation of monitoring tools and control strategies in order to produce a desired product with its corresponding target properties. Application of the framework is highlighted through a case study involving the system potassium dihydrogen phosphate (KDP), for which the targeted CSD is defined and achieved in one- and two-dimensional schemes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Abdul Samad, N. A. F. B. (Intern), Meisler, K. T. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2012

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Title of host publication: Proceedings of the 22nd European Symposium on Computer Aided Process Engineering
Chapter: 5
Main Research Area: Technical/natural sciences

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
Authors: Abdul Samad, N. A. F. B. (Intern), Meisler, K. T. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Process monitoring and control, Analytical estimator, Crystal distribution, Crystal shape

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A generic process template for continuous pharmaceutical production

In the work reported here, a conceptual generic continuous process template for pharmaceutical production is presented. The template is demonstrated on a nitro reduction case study that should in principle be generic such that it can handle a series of substrates with similar molecular functionality. To assist in adoption of different substrates, a systematic substrate adoption methodology (SAM) has also been developed. The objective of the generic process template together with the SAM is to provide flexibility as well as increased efficiency to continuous processes while reducing inventory for
safer operations (from 50 to 100 L in batch or 3 to 5 L in continuous processes). It is shown that the use of the template
together with SAM can lead to potential savings in product development times through flexible and efficient production of
Kg amounts of product material for clinical trials and other analyses.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology,
Computer Aided Process Engineering Center, AstraZeneca
Authors: Singh, R. (Intern), Rozada-Sanches, R. (Ekstern), Dean, W. (Ekstern), Perkins, J. (Ekstern), Muller, F. (Ekstern),
Godfrey, A. (Ekstern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
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A generic process template for continuous pharmaceutical production

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology,
Computer Aided Process Engineering Center, AstraZeneca
Authors: Singh, R. (Intern), Rozada-Sanches, R. (Ekstern), Dean, W. (Ekstern), Perkins, J. (Ekstern), Muller, F. (Ekstern),
Godfrey, A. (Ekstern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research › Poster – Annual report year: 2012

A model-data based systems approach to process intensification
In recent years process intensification (PI) has attracted much interest as a potential means of process improvement to
meet the demands, such as, for sustainable production. A variety of intensified equipment are being developed that
potentially creates options to meet these demands. Their developments, however, are largely due to experiment based
trial and error approaches and while they do not require validation, they can be time consuming and resource intensive.
Also, one may ask, can a truly new intensified unit operation be obtained in this way? An alternative two-stage approach is
to apply a model-based synthesis method to systematically generate and evaluate alternatives in the first stage and an
experiment-model based validation in the second stage. In this way, the search for alternatives is done very quickly,
reliably and systematically over a wide range, while resources are preserved for focused validation of only the promising
candidates in the second-stage. This approach, however, would be limited to intensification based on “known” unit
operations, unless the PI process synthesis/design is considered at a lower level of aggregation, namely the phenomena
level. That is, the model-based synthesis method must employ models at lower levels of aggregation and through
combination rules for phenomena, generate (synthesize) new intensified unit operations. An efficient solution procedure
for the synthesis problem is needed to tackle the potentially large number of options that would be obtained. Here,
established procedures for computer aided molecular design is adopted since combination of phenomena to form unit
operations with desired objectives is, in principle, similar to combining atoms to form molecules with desired properties.
The concept of the phenomena-based synthesis/design method for process intensification will be presented together with
illustrations of its application through case studies. Aspects such as need for models, computer-aided framework, the
work-flow and data-flow for the PI synthesis method will also be highlighted.
A model-data based systems approach to process intensification

In recent years process intensification (PI) has attracted much interest as a potential means of process improvement to meet the demands, such as, for sustainable production. A variety of intensified equipment are being developed that potentially creates options to meet these demands. Their developments, however, are largely due to experiment based trial and error approaches and while they do not require validation, they can be time consuming and resource intensive. Also, one may ask, can a truly new intensified unit operation be obtained in this way? An alternative two-stage approach is to apply a model-based synthesis method to systematically generate and evaluate alternatives in the first stage and an experiment-model based validation in the second stage. In this way, the search for alternatives is done very quickly, reliably and systematically over a wide range, while resources are preserved for focused validation of only the promising candidates in the second-stage. This approach, however, would be limited to intensification based on “known” unit operations, unless the PI process synthesis/design is considered at a lower level of aggregation, namely the phenomena level. That is, the model-based synthesis method must employ models at lower levels of aggregation and through combination rules for phenomena, generate (synthesize) new intensified unit operations. An efficient solution procedure for the synthesis problem is needed to tackle the potentially large number of options that would be obtained. Here, established procedures for computer aided molecular design is adopted since combination of phenomena to form unit operations with desired objectives is, in principle, similar to combining atoms to form molecules with desired properties. The concept of the phenomena-based synthesis/design method for process intensification will be presented together with illustrations of its application through case studies. Aspects such as need for models, computer-aided framework, the work-flow and data-flow for the PI synthesis method will also be highlighted.

A New Paradigm for Chemical Engineering?

One of the major concerns facing the world today arises from increasing industrial activities that have lead to rapid depletion of non-renewable resources and increase in pollution. With the current emphasis on sustainability, much improvement is expected from the process industry to minimize raw material, energy usage and waste generation without compromising the economic value of the enterprise. Responding to these challenges requires a new insight into the characteristics of a sustainable system, for example, how to incorporate the product, the process and the related supply chain within the system boundary under investigation? A fundamental rethinking of how to identify the needed chemicals based products and how to design, build and operate the corresponding production units, is necessary. Indeed, the chemical industry today is changed from the chemical industry of forty years ago. Clear evidence of this change comes from the jobs taken by graduating chemical engineering professionals in North America, Europe, and some of the Asian countries. In terms of where the graduating chemical engineers are going to work, a clear shift from the commodity chemical industry to the product oriented businesses has been observed. There is an increasing trend within the chemical industry to focus on products and the sustainable processes that can make them. Do these changes point to a paradigm shift in chemical engineering as a discipline? Historically, two previous paradigm shifts in chemical engineering corresponded to major shifts in chemical engineering as a discipline, which affected not only the education of chemical engineers, but also the development of chemical engineering as a discipline. Has the time come for a new paradigm shift that will prepare the current and future chemical engineering graduates to tackle the complex problems facing the chemicals based industries and serve the modern society more efficiently? The lecture will review the current status of chemical engineering as a discipline, the proposals for the third paradigm, the need for such a paradigm shift and related educational issues.
An Integrated Methodology for Design of Tailor-Made Blended Products

A computer-aided methodology has been developed for the design of blended (mixture) products. Through this methodology, it is possible to identify the most suitable chemicals for blending, and “tailor” the blend according to specified product needs. The methodology has three stages: 1) product design, 2) process identification, and 3) experimental verification. The principle problem, which is the product design stage is divided into four sub-problems and solved with a decomposition-based approach. In stage two, the ability to produce the chemicals used as building blocks in the blends is analyzed. Finally, experimental work (or detailed model-based verification) is conducted in stage three to validate the selected blend candidates. In this study, the product design stage is highlighted through a case study of gasoline blends with bio-based chemicals. The objective of this study is to identify blended gasoline products that match (or improve) the performance of the conventional gasoline.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
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Conference: 22nd European Symposium on Computer Aided Process Engineering, London, United Kingdom, 17/06/2012 - 17/06/2012
Product design, Chemical blends, Decomposition method, Gasoline
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An Integrated Methodology for Design of Tailor-Made Blended Products

An important issue for the production of many chemical-based products is related to the future supply of the essential raw materials. Currently, many of these products are derived from fossil fuel based raw materials and from a sustainability point of view, other renewable alternatives need to be considered. In order to achieve this, new products need to be developed by blending the conventional materials with other chemicals that can be produced from renewable resources, such as bio-based chemicals. Blending could offer several advantages, such as, reducing the amount of fossil fuel consumption, decreasing the pollution level and increasing the product safety. In addition, potentially the product attributes also can be improved by blending. However, the product performance may decline when other chemicals are added. In order to maintain/improve the blended product performance, it is necessary to identify the best product blend with the most appropriate chemicals. Therefore, an integrated methodology to design mixture/blend products is developed, which is able to find the most suitable chemicals for blending, and produce blended products that satisfy specific product needs. The methodology has three stages: 1) product design, 2) process identification, and 3) experimental verification. At the first stage, a computer-aided methodology is implemented to quickly identify and evaluate the most promising blend candidates. In this paper, the product design issues are highlighted considering only chemicals from known bio-based sources. The product design stage has four tasks. First, the design problem is defined where the product needs are identified, translated into target properties and given target values. Secondly, target property models are retrieved from a property model library
developed specifically for this methodology. Thirdly, a mixture/blend design algorithm is applied to obtain the mixtures/blends that match the set of constraints (design targets). This algorithm employs a decomposition based solution strategy to solve the mixture/blend problem. The result is a set of blends that match the constraints, the compositions, values of the target properties and information about their miscibility. Finally, the mixture target property values are verified either with experimental data (if available) or by means of rigorous models for the properties and mixtures that require it. The application of this systematic methodology is highlighted through case studies related to the design of blended gasoline, lubricants and refrigerants, where the objective is to identify blended products that satisfy all the product attributes with at least similar or better performance compared to conventional products.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Number of pages: 1
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Main Research Area: Technical/natural sciences
Chemicals based products, Chemical blends, product design, Computer-aided approach
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Publication: Research › Conference abstract for conference – Annual report year: 2012

An Integrated Methodology for Design of Tailor-Made Blended Products
General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research › Poster – Annual report year: 2012

An Integrated Methodology for Design of Tailor-Made Blended Products: Biofuels and Bio-Based Lubricants

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
Authors: Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Paper 546a.pdf
Links:
https://aiche.confex.com/aiche/2012/webprogram/Paper264319.html

Bibliographical note
Oral presentation.
Source: dtu
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Application of the UNIFAC-CI Model for Phase Equilibria Predictions of Organic Chemical System

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Mustaffa, A. A. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Are safe results obtained when SAFT equations are applied to ordinary chemicals?: Part 2: Study of solid–liquid equilibria in binary systems

In a previous work, some irregular behaviours of the PC-SAFT EoS – and more generally of SAFT-type EoS – were pointed out for pure components at low temperatures. In particular, it was shown that for pure fluids at a fixed temperature and pressure, these equations of state were likely to exhibit up to five molar volumes, thus leading to the simultaneous existence of pseudo liquid–liquid and liquid–vapour phase equilibria at a same temperature. In this work, low-temperature calculations are performed using the PC-SAFT EoS which is combined with a fugacity model for the solid phase in order to predict solid–liquid phase equilibria. It is shown that when varying the binary-interaction parameter of the PC-SAFT equation, non-feasible phase diagrams may be calculated including for instance, the presence of a liquid–liquid azeotrope, of a liquid–liquid–solid–solid four-phase equilibrium or the simultaneous existence of several eutectic points.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Université de Lorraine
Authors: Privat, R. (Ekstern), Conte, E. (Intern), Jaubert, J. (Ekstern), Gani, R. (Intern)
Pages: 61-76
Publication date: 2012
Main Research Area: Technical/natural sciences

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Volume: 318
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Effective estimation of parameters in biocatalytic reaction kinetic expressions are very important when building process models to enable evaluation of process technology options and alternative biocatalysts. The kinetic models used to describe enzyme-catalyzed reactions generally include several parameters, which are strongly correlated with each other. State-of-the-art methodologies such as nonlinear regression (using progress curves) or graphical analysis (using initial rate data, for example, the Lineweaver-Burke plot, Hanes plot or Dixon plot) often incorporate errors in the estimates and rarely lead to globally optimized parameter values. In this article, a robust methodology to estimate parameters for biocatalytic reaction kinetic expressions is proposed. The methodology determines the parameters in a systematic manner by exploiting the best features of several of the current approaches. The parameter estimation problem is decomposed into five hierarchical steps, where the solution of each of the steps becomes the input for the subsequent step to achieve the final model with the corresponding regressed parameters. The model is further used for validating its performance and determining the correlation of the parameters. The final model with the fitted parameters is able to describe both initial rate and dynamic experiments. Application of the methodology is illustrated with a case study using the x-transaminase catalyzed synthesis of 1-phenylethylamine from acetophenone and 2-propylamine.
A Systematic Approach for Optimized Water Allocation Through Solution of Large Scale Water/Wastewater Networks Problems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Quaglia, A. (Intern), Pennati, A. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Paper 246e.pdf
Links:
https://aiche.confex.com/aiche/2012/webprogram/Paper278824.html

A Systematic Framework for Synthesis and Design of Multi-Scale Processing Networks Using Incremental-Based Solution Strategy

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Shishmarev, M. (Ekstern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Paper 534c.pdf
Links:
https://aiche.confex.com/aiche/2012/webprogram/Paper267625.html

A Systematic Methodology for Design of Emulsion Based Chemical Products
A systematic methodology for emulsion based chemical product design is presented. The methodology employs a model-based product synthesis/design stage and a modelexperiment based further refinement and/or validation stage. In this paper only the first stage is presented. The methodology employs a hierarchical approach starting with the identification of the needs to be satisfied by the emulsified product and then building up the formulation by adding one-by-one the different classes of chemicals. A structured database together with dedicated property prediction models and evaluation criteria are employed to obtain a list of formulations that satisfy constraints representing the desired needs (target properties). Through a conceptual case study dealing with the design of a sunscreen lotion, the application of this new methodology is illustrated.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Pages: 220-224
A Systematic Methodology for Design of Emulsion Based Chemical Products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
PSE_2012_Poster.pdf
Source: dtu
Source-ID: u::4752
Publication: Research › Poster – Annual report year: 2012

A systems engineering approach to manage the complexity in sustainable chemical product-process design

This paper provides a perspective on model-data based solution approaches for chemical product-process design, which consists of finding the identity of the candidate chemical product, designing the process that can sustainably manufacture it and verifying the performance of the product during application. The chemical product tree is potentially very large and a wide range of options exist for selecting the product to make, the raw material to use as well as the processing route to employ. It is shown that systematic computer-aided methods and tools integrated within a model-data based design framework can manage the complexity associated with product-process problems very efficiently. Three specific computer-aided tools (ICAS, Sustain-Pro and VPPDLab) have been presented and their applications to product-process design, highlighted.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Number of pages: 15
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
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Source-ID: u::4270
Publication: Research › Paper – Annual report year: 2012

A systems engineering approach to manage the complexity in sustainable chemical product-process design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Number of pages: 1
Carbon Dioxide Capture Processes: Sensitivity Analysis for Optimization and Control

Carbon dioxide is the main greenhouse gas and its major source is combustion of fossil fuels for power generation. The objective of this study is to carry out the steady-state sensitivity analysis for chemical absorption of carbon dioxide capture from flue gas using monoethanolamine solvent. First a consistent simulation of the process verifying a base case design has been performed. Available commercial simulation package Aspen Plus 7.2 is used for the steady state simulations. An equilibrium based model for the process simulations together with the electrolyte-NRTL model for the vapor liquid equilibrium and associated property models are used. Simulations are performed to investigate the sensitivity of the process variables to change in the design variables including process inputs and disturbances in the property model parameters. Results of the sensitivity analysis on the steady state performance of the process to the L/G ratio to the
absorber, CO2 lean solvent loadings, and striper pressure are presented in this paper. Based on the sensitivity analysis process optimization problems have been defined and solved and, a preliminary control structure selection has been made.

**General information**
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Korea Advanced Institute of Science & Technology
- **Authors:** Zaman, M. (Ekstern), Lee, J. H. (Ekstern), Gani, R. (Intern)
- **Pages:** 539-544
- **Publication date:** 2012

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- **Publisher:** IEEE
- **ISBN (Print):** 978-1-4673-2247-8
- **Main Research Area:** Technical/natural sciences
- **Conference:** 12th International Conference on Control, Automation and Systems, Jeju Island, Korea, Republic of, 17/10/2012 - 17/10/2012
- **Carbon dioxide capture, Chemical absorption, Sensitivity analysis, Operability and control**
- **Source:** dtu
- **Source-ID:** n::oai:DTIC-ART:iel/377141945::24412
- **Publication: Research - peer-review › Article in proceedings – Annual report year: 2012**

**Computer-aided approach for design of tailor-made blended products**

**General information**
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
- **Authors:** Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
- **Publication date:** 2012
- **Event:** Abstract from 3rd International Gas Processing Symposium, Doha, Qatar.
- **Main Research Area:** Technical/natural sciences
- **Computer-aided approach, Chemical blends, Product design, Gasoline, Refrigerant**
- **Electronic versions:**
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- **Oral presentation**
- **Source:** dtu
- **Source-ID:** u::4260
- **Publication: Research › Conference abstract for conference – Annual report year: 2012**

**Computer-aided approach for design of tailor-made blended products**

A computer-aided methodology has been developed for the design of blended (mixture) products. Through this methodology, it is possible to identify the most suitable chemicals for blending, and “tailor” the blend according to specified product needs (usually product attributes, e.g. performance as well as regulatory). The product design methodology has four tasks. First, the design problem is defined: the product needs are identified, translated into target properties and the constraints for each target property are defined. Secondly, target property models are retrieved from a property model library developed specifically for this methodology. Thirdly, a mixture/blend design algorithm is applied to obtain the mixtures/blends (gasoline blend in this case) that match the set of constraints (design targets). The result is a set of blends that match the constraints, the composition of the chemicals present in the blend, values of the target properties and information about their miscibility. Finally, the mixture target property values are verified by means of rigorous models for the properties and mixtures. The application of this systematic methodology is highlighted through case studies related to the design of blended gasoline with different types of blending agents. The objective of this study is to identify blended gasoline products that match the traditional gasoline attributes and identify suitable blending agents for gasoline.

**General information**
- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology
- **Authors:** Yunus, N. A. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
- **Pages:** 303-310
Consistent Prediction of Properties of Systems with Lipids

Equilibria between vapour, liquid and/or solid phases, pure component properties and also the mixture-phase properties are necessary for synthesis, design and analysis of different unit operations found in the production of edible oils, fats and biodiesel. A systematic numerical analysis is employed to determine the needs of phase equilibria and related properties in processes such as Deodorization, Dry Fractionation, Solvent Extraction and Biodiesel Production. Other important use for the data and analysis is in property model development for correct and consistent property prediction. Lipids are found in almost all mixtures involving edible oils, fats and biodiesel. They are also being extracted for use in the pharma-industry.

A database for pure components (lipids) present in these processes and mixtures properties has been developed and made available for different applications (model development, property verification, property prediction, etc.). The database has verified data for fatty acids, acylglycerols, fatty esters, fatty alcohols, vegetable oils, biodiesel and minor compounds as phospholipids, tocopherols, sterols, carotene and squalene, together with a user friendly interface that allows an easy search/retrieve of the data (pure component and mixture properties). In total, there are 240 different pure compounds, 229 different phase equilibrium systems (72 VLE, 85 LLE, 72 SLE), 63 solubility systems, and around 4500 data points on phase equilibria. Critical properties, enthalpy of formation, heats of combustion, heats of fusion, normal melting point, normal boiling point, and also temperature dependent properties such as vapour pressure, liquid enthalpy, heats of vaporization, liquid density, liquid viscosity and surface tension are present. Also the parameters for different well-known thermodynamic models (UNIFAC, UNIQUAC, NRTL) have been added to the database. There is a parameter regression option for those systems for which model parameters have not been reported but experimental data can be found in the literature. The well-known property models have been further extended with group-contribution combined with atom connectivity based models. Some of these models are UNIFAC-CI, PC-SAFT (for pure component properties only) and the NRTL-SAC. In this paper, details of the data available in the database together with an analysis of the data will be presented. The analysis checks for consistency of pure component properties and their use in mixture properties. Thermodynamic consistency tests such as the Van Ness Test, Herrington Test (Area Test), Point Test (Differential Test) and Infinite Dilution Test have also been performed. Based on the analysis, an uncertainty score is given, which is then used to define the weights of data-sets to be used for property model parameter regression. The performance of selected models for pure component properties as well as mixture properties when applied to systems containing lipids will be highlighted.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, State University of Campinas, Alfa Laval Copenhagen A/S
Authors: Cunico, L. (Intern), Ceriani, R. (Ekstern), Sarup, B. (Ekstern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from ESAT 2012, Potsdam, Germany.
Main Research Area: Technical/natural sciences

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

Control of Process Operations and Monitoring of Product Qualities through Generic Model-based Framework in Crystallization Processes
A generic and systematic model-based framework for the design of a process monitoring and control system to achieve the desired crystal size distribution (CSD) and crystal shape for a wide range of crystallization processes has been developed. This framework combines a generic multi-dimensional modelling framework, tools for design of set point profiles, for design of PAT (Process Analytical Technology) systems as well as option to perform the uncertainty and sensitivity analysis of the PAT system design. Through this framework, it is possible for a wide range of crystallization processes to generate the necessary problem-system specific model, the necessary set point using the extended analytical CSD estimator and the response surface method (RSM) and a PAT system design including implementation of monitoring tools and control strategies in order to produce a desired product with its corresponding target properties. In addition the impact and influence of input uncertainties on the predicted PAT system performance can be quantified, i.e. the risk of not achieving the target specifications of the crystal product can also be investigated. The application of the systematic model-based framework is divided into three sections: a) the application of the generic multi-dimensional modelling framework are highlighted: i) the capability to develop and further extend a batch cooling crystallization model is illustrated through a paracetamol case study, supplemented by a sucrose crystallization example to demonstrate how the framework supports smooth switching between chemical systems with a minimum modelling effort; ii) a potassium dihydrogen phosphate (KDP) case study is used to demonstrate how the model complexity can be increased, that is, by switching from a one-dimensional to a twodimensional description; b) the systematic framework is used in a case study to design a monitoring and control (PAT) system for a potassium dichromate and KDP crystallization processes to achieve the desired target CSD respectively; and c) Based on the PAT system design in b), the application of uncertainty and sensitivity analysis is then highlighted for the potassium dichromate and KDP crystallization process both in open-loop and closed-loop operation. In the case study, the impact of input uncertainties related to parameters of the nucleation and the crystal growth model on the predicted system performance has been investigated for a one- and two-dimensional CSD and it shown the PAT system design is reliable and robust under considered uncertainties.

**General Information**

State: Published

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

Authors: Abdul Samad, N. A. F. B. (Intern), Gani, R. (Intern), Gernaey, K. (Intern), Sin, G. (Intern)

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Main Research Area: Technical/natural sciences

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Publication: Research › Ph.D. thesis – Annual report year: 2012

**Design methodology for bio-based processing: Biodiesel and fatty alcohol production**

A systematic design methodology is developed for producing two main products plus side products starting with one or more bio-based renewable source. A superstructure that includes all possible reaction and separation operations is generated through thermodynamic insights and available data. The number of alternative processes is systematically reduced through a screening procedure until only feasible alternatives are obtained. As part of the methodology, process intensification involving reaction-separation tasks is also considered to improve the design by shifting the equilibrium reactions. Economic analysis and net present value are determined to find the best economically and operationally feasible process. The application of the methodology is presented through a case study involving biodiesel and fatty alcohol productions.

**General Information**

State: Published

Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Chulalongkorn University

Authors: Simasatikul, L. (Ekstern), Arpornwichanop, A. (Ekstern), Gani, R. (Intern)

Pages: 855-859
Design of an Emulsified Hand Wash Through a Systematic Model-Based Methodology

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Columbia University
Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_176c.pdf
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Source: dtu
Source-ID: u::4483
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Design of Formulated Products: Experimental Component

A systematic methodology for the design and verification of chemical-based products is proposed. By integrating modeling, and experiments, the search space is efficiently scanned to identify the feasible product candidates. The product design (or verification) problem consists of three stages: computer-aided design (Stage 1), which generates a list of feasible candidates, experimental planning (Stage 2), which generates a list of experiments and checks the available experimental set-ups, and experimental testing (Stage 3), which measures the necessary data and verifies the desirable attributes of the final product. The first stage (Stage 1) has been covered in previous publications, along with detailed case studies. The development of Stage 2 and Stage 3 is considered in this article and highlighted through two case studies involving the design and validation of an insect repellent lotion and a sunscreen lotion.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Gani, R. (Intern), Cheng, Y. S. (Ekstern), Ng, K. M. (Ekstern)
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Insect repellent lotion, Product design, Experimental testing, Sunscreen lotion, Formulation design

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10.1002/aic.12582
Development and Analysis of Original UNIFAC-CI and Modified UNIFAC-CI Models for Prediction of VLE and SLE Systems

Prediction of properties is important in chemical process-product design. Group-contribution (GC) methods provide a useful tool but there is a need to validate and improve their accuracy when complex chemicals are present in the mixtures. In accordance with that, a combined GC and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties. This so-called GCPlus approach is a hybrid model which combines GC and valence connectivity indices (CI). The main idea is the use of CI to describe the molecular fragmentation that relates properties, the molecular interactions with the molecular structures. One established GC method is the UNIFAC model to predict liquid phase activity coefficients. The needed values of the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, values of the missing GIPs, can be predicted through the GCPlus approach. The predicted values for the GIPs are then used in the UNIFAC model to calculate activity coefficients. In this work, the model parameters for using the GCPlus approach to the original UNIFAC and Modified (Dortmund) UNIFAC have been regressed against vapor-liquid equilibrium (VLE) data and simultaneously against VLE and solid-liquid equilibrium (SLE) data for groups formed by C, H, O, N, Cl and S atoms. Initially the VLE data used to regress those parameters are checked using a quality assessment algorithm which combines four widely used consistency tests (Herington, Van Ness, Point/Differential and Infinite Dilution tests) and also a check on the consistencies of the data with the pure component vapor pressures. The overall quality factors, QVLE obtained for each dataset indicate the quality of each datasets and can then be used as weighting factors, in the objective function for the parameter regression with VLE data (and with SLE data). The performance of the CI-models using parameters regressed against VLE data and simultaneously against VLE and SLE data are compared in terms of the uncertainties of the parameters regressed against the predicted properties and the accuracy of the predictions. In addition, the model performances are compared with their reference UNIFAC models.
Editorial note: Best paper of 2010 award

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Purdue University
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Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
Effect of Uncertainties in Physical Property Estimates on Process Design - Sensitivity Analysis

Chemical process design calculations require accurate and reliable physical and thermodynamic property data and property models of pure components and their mixtures in order to obtain reliable design parameters which help to achieve desired specifications. The uncertainties in the property values can arise from the experiments itself or from the property models employed. It is important to consider the effect of these uncertainties on the process design in order to assess the quality and reliability of the final design. The main objective of this work is to develop a systematic methodology for performing sensitivity of process design subject to uncertainties in the property estimates. To this end, first uncertainty analysis of the property models of pure components and their mixtures was performed in order to obtain the uncertainties in the estimated property values. As a next step, sensitivity analysis was performed to evaluate the effect of these uncertainties on the process design. The developed methodology was applied to evaluate the effect of uncertainties in the property estimates on design of different unit operations such as extractive distillation, short path evaporator, equilibrium reactor, liquid-liquid extraction, crystallizer etc. The sensitivity of design parameters to uncertainties in the property estimates was performed using one-factor-at-a-time approach. The results showed that depending on the pure components and their mixtures involved, the driving forces they represented, the operating conditions, and the choice of the property prediction models, the input uncertainties resulted in significant uncertainties in the final design. The developed methodology was able to: (i) assess the quality of final design; (ii) identify pure component and mixture properties of critical importance from a process design point-of-view; (iii) identify additional experimentation needs to reduce the most critical uncertainties; and (iv) establish acceptable levels of accuracy for property prediction models employed.

General information

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CAPEC-PROCESS
Authors: Hukkerikar, A. (Intern), Jones, M. N. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 1
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Main Research Area: Technical/natural sciences
Electronic versions: AMH_ThermoSymposium_Abstract_2.pdf
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-contribution+ (GC+) method (combined group-contribution (GC) method and atom connectivity index (CI)) based 15 property models to provide reliable estimations of environment-related properties of organic chemicals together with uncertainties of estimated property values. For this purpose, a systematic methodology for property modeling and uncertainty analysis is used. The methodology includes a parameter estimation step to determine parameters of property models and an uncertainty analysis step to establish statistical information about the quality of parameter estimation, such as the parameter covariance, the standard errors in predicted properties, and the confidence intervals. For parameter estimation, large data sets of experimentally measured property values of a wide range of chemicals (hydrocarbons, oxygenated chemicals, nitrogenated chemicals, polyfunctional chemicals, etc.) taken from the database of the US Environmental Protection Agency (EPA) and from the database of USEtox is used. For property modeling and uncertainty analysis, the Marrero and Gani GC method and atom connectivity index method have been considered. In total, 22 environment-related properties, which include the fathead minnow 96-h LC50, Daphnia magna 48-h LC50, oral rat LD50, aqueous solubility, bioconcentration factor, permissible exposure limit (OSHA- TWA), photochemical oxidation potential, global warming potential, ozone depletion potential, acidification potential, emission to urban air (carcinogenic and noncarcinogenic), emission to continental rural air (carcinogenic and noncarcinogenic), emission to continental fresh water (carcinogenic and noncarcinogenic), emission to continental seawater (carcinogenic and noncarcinogenic), emission to continental natural soil (carcinogenic and noncarcinogenic), and emission to continental agricultural soil (carcinogenic and noncarcinogenic) have been modeled and analyzed. The application of the developed property models for the estimation of environment-related properties and uncertainties of the estimated property values is highlighted through an illustrative example. The developed property models provide reliable estimates of environment-related properties needed to perform process synthesis, design, and analysis of sustainable chemical processes and allow one to evaluate the effect of uncertainties of estimated property values on the calculated performance of processes giving useful insights into quality and reliability of the design of sustainable processes.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S, National Risk Management Research Laboratory, Chulalongkorn University
Authors: Hukkerikar, A. (Intern), Kalakul, S. (Ekstern), Sarup, B. (Ekstern), Young, D. M. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 2823-2839
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.647 SNIP 1.345 CiteScore 4.4
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Web of Science (2013): Indexed yes
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Physical and thermodynamic properties of pure components are needed to carry out tasks such as process design and computer aided molecular/mixture design among others. The experimental values of properties of many important pure components have not been measured due to many reasons, and hence they must be estimated. Predictive methods such as the group-contribution+ (GC+) method (combined group-contribution (GC) method and atom connectivity index (CI) method) are generally suitable to estimate the needed property values. For assessing the quality and reliability of the selected property prediction method, an engineer needs to know the uncertainties in the estimated property values obtained from that method. With this information, the engineer can then perform better-informed design calculations by taking into account these uncertainties. Hence, given the importance of reliable estimation of properties and uncertainties in the property estimates in the engineering calculations, this work aims to revise and improve GC+ method based estimation of properties as well as to estimate the confidence intervals of estimated property values. To this end, a systematic methodology for property modeling and uncertainty analysis, in general, is developed and used. In total 21 properties of pure components, which include normal boiling point, critical constants, normal melting point among others have been analysed. The statistical analysis of the model performance for these properties is highlighted through several illustrative examples. Important issues related to property modeling such as thermodynamic consistency of the predicted properties (relation of normal boiling point versus critical temperature etc.) are analysed. The developed methodology is simple, yet sound and effective and provides not only the estimated property values using the GC+ approach, but also the uncertainties in the estimated property values. This feature allows one to evaluate the effects of these uncertainties on the product-process design calculations thereby contributing to better-informed and reliable engineering solutions.
Framework for the analysis of crystallization operations

Crystallization is often applied in the production of salts and/or active pharmaceutical ingredients (API), and the crystallization step is an essential part of the manufacturing process for many chemicals-based products. In recent years, the monitoring and analysis of crystallization operations has received increased attention due to the growing need to control more sophisticated production lines as well as to measure/monitor the final product characteristics.

Crystallization operations involve a combination of several phenomena, and different kinetic models are required for their modeling. Growth of the crystals occurs in multiple dimensions and the relative rates of different growth and other kinetic phenomena control the shape and size distribution of the final product. Including several dimensions in the crystallization will allow a more general description of the kinetic phenomena and the crystallization operation. In order to have a full description of a crystallizer, a combination of constitutive (kinetic) models is needed. Development of appropriate constitutive models requires data, which for size distributions in crystallization operations is available in the form of chord length distribution data (from Focused Beam Reflectance Measurements (FBRM)). Use of this data for modeling requires a data translation procedure.

The objective of this paper is to present a modeling procedure for systematic development of constitutive models for use in design, analysis, and simulation of crystallization operations. This procedure has three main features: A data handling and translation feature, a constitutive model identification feature, and a model application feature. For different crystallization operation scenarios, the measured data is translated to create an image of the product. Through the model identification option, the parameters of the constitutive models embedded within the crystallizer model are regressed to match the translated product image. With the models identified, they are applied to understand, design and/or analyze various crystallization operational scenarios.

The paper will present the constitutive model development procedure as part of a general crystallization modeling framework. It will highlight the different features through a case study involving measured data and use it to develop models and finally, the use of the model to analyze different crystallization operations.
Group Contribution+ (GC+) Based Estimation of Environment-Related Properties for Design of Sustainable Processes: Development of Property Models and Uncertainty Analysis

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S, National Risk Management Research Laboratory
Authors: Hukkerikar, A. (Intern), Sarup, B. (Ekstern), Young, D. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S, Akzo Nobel Functional Chemicals AB
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Pages: 25-43
Publication date: 2012
Main Research Area: Technical/natural sciences
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.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
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Integrating Porous Resins In Enzymatic Processes

Increasing pressure mandated by different government policies, for developing sustainable chemical processes for the synthesis of optically pure compounds, has resulted in increased considerations of biocatalysis as a viable option by many industries. Biocatalysis, with its exquisite selective properties and potential ‘green’ attributes, presents it as a sustainable alternative. Today, the role of biocatalysis is most evident in the pharmaceutical industry and is currently extending towards fine and bulk chemical production as well. The use of hydrolytic enzymes (lipases) is well established in several chemical industries, though certain challenges persist in other types of enzymes (transferases and ketoreductases), thus limiting their implementation in industry. Inhibition by substrate and product as well as low aqueous solubility of substrates has constrained the full potential of these enzymes to be harnessed. Porous resins as opposed to other auxiliary phases, for example organic solvents, are nonbioavailable, biocompatible and offer simpler operational handling (no foaming and emulsification). This strategy has been applied effectively to single substrate – single product systems (oxidation, V microbial degradation and hydrolysis). However, this concept has not been extended to other industrially relevant reactions which are two substrate – two product systems. In this thesis, a methodological framework has been successfully developed to aid in implementing the strategy of integrating porous resins for multi-component systems. In this manner, a generic platform has been established for biocatalytic reactions that require the integration of this strategy. The framework identifies the key information about the reaction and the process using a step-wise protocol with the required tools. It includes the use of kinetic modelling in characterizing the reaction kinetics, a heuristic approach for screening resins and a model based approach for evaluating the process. Greater knowledge about the enzymatic processes with integrated porous resins can therefore be gained and thus the efficiency of process development with respect to time and resources required (reduced number of experiments) could be increased. Estimating kinetic model parameters for enzymatic reactions is quite complex and frequently leads to identifiability issues. In order to understand the different techniques to estimate the parameters, a number of concepts are discussed in chapter four of this thesis. This
knowledge has contributed to the development of a robust methodology for the estimation of kinetic model parameters for biocatalytic reactions, which has also been published in a peer reviewed journal. Screening resins for moderately hydrophobic multi-component systems is challenging. Often it is found that the capacity of the resin is inversely related with product selectivity. Therefore a tradeoff has to be made between these parameters which can be crucial from an economic point of view. A low resin capacity points towards the need for higher resin loading, which in turn determines the equilibrium concentration of the substrate in the reactor and the type of reactor that can be used (stirred tank reactor or packed bed reactor). Similarly low product selectivity would result in higher product concentration in the reactor and thus not aid in alleviating inhibition. Further considerations include as process modelling is a very effective tool in evaluating a process. Critical information about the process can be gained by means of simulations, which can further be re-used to tune the reaction or process conditions to harness the full potential of the enzyme. State-of-the-art mathematical techniques for model quality evaluation, such as uncertainty and sensitivity analysis, have been included in this analysis in order to identify the key model parameters for better understanding of the process. Three case studies were used to illustrate the applicability of the methodology to fulfil different objective requirements. The case studies were selected for not only being industrially relevant but as well as having certain limitations which contributed in developing the tools and strategies to overcome them. The asymmetric synthesis of 1-phenylethylamine using \textit{-}transaminise, the asymmetric synthesis of 1-methyl-3-phenylpropylamine using \textit{-}transaminise and enantioselective synthesis of 2-octanol using alcohol dehydrogenase were selected. VI of resin stability and cost also have to be taken into account in the screening procedure. The screening therefore becomes a multi-objective task that has to be solved simultaneously. Such an approach has been applied in the method formulated in this framework.

To overcome these challenges, different process strategies are required to obtain high yields. A number of different challenges and proposed solutions are discussed in chapter one of this thesis and have also been published as a review. In recent years, integrating porous resins as an auxiliary phase in enzymatic processes, to non-selectively bind the substrate and product as a means to alleviate substrate and product inhibition, has gained considerable recognition. The resins act as a reservoir for the inhibitory substrate and a sink for the inhibitory product and simultaneously attain the required high substrate loading to make the process economically feasible. In this way the potential benefit of the enzyme can be exploited.

**General information**

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Organisations: Center for Process Engineering and Technology, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center  
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**Modelling of physical properties - databases, uncertainties and predictive power**

Physical and thermodynamic property in the form of raw data or estimated values for pure compounds and mixtures are important pre-requisites for performing tasks such as, process design, simulation and optimization; computer aided molecular/mixture (product) design; and, product-process analysis. While use of experimentally measured values of the needed properties is desirable in these experiments, the experimental data of the properties of interest may not be available or may not be measurable in many cases. Therefore, property models that are reliable, predictive and easy to use are necessary. However, which models should be used to provide the reliable estimates of the required properties? And, how much measured data is necessary to regress the model parameters? How to ensure predictive capabilities in the developed models? Also, as it is necessary to know the associated uncertainties in the estimated/predicted property values, how to assess the quality and reliability of the estimated/predicted property values?

The paper will review a class of models for prediction of physical and thermodynamic properties of organic chemicals and their mixtures based on the combined group contribution – atom connectivity approach. The development of these models requires measured property data and based on them, the regression of model parameters is performed. Although this class of models is empirical by nature, they do allow extrapolation from the regressed model parameters to predict properties of chemicals not included in the measured data-set. Therefore, they are also considered as predictive models.
The paper will highlight different issues/challenges related to the role of the databases and the mathematical and thermodynamic consistency of the measured/estimated data, the predictive nature of the developed models, the uncertainty estimates of the predicted data. Related to the database, the consistency of the collected data, the uncertainties in the measured values, and the amount of data to be used in the regression step, will be discussed and analyzed. Related to modelling, the predictive nature of the models, the calculation of the uncertainties of the estimated property values, the theoretical trends will be illustrated with examples.

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**Molecular structure based physical properties modelling**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
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Event: Abstract from MTMS’12, Higashi-Hiroshima, Japan.
Main Research Area: Technical/natural sciences
Property prediction, Molecular structure, Group contribution-connectivity index
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**NIST ThermoData Engine: Extension to Solvent Design and Propagation of Uncertainties for Process Simulation**

NIST ThermoData Engine (TDE, NIST Standard Reference Databases 103a and 103b) is the first product that implements the concept of Dynamic Data Evaluation in the fields of thermophysics and thermochemistry, which includes maintaining the comprehensive and up-to-date database of experimentally measured property values and expert system for data analysis and generation of recommended property values at the specified conditions along with uncertainties on demand. The most recent extension of TDE covers solvent design and multi-component process stream property calculations with uncertainty analysis.

Solvent Design function serves three tasks: (1) selection of best solvent for a solid solute, (2) search for a selective solvent for a solid binary mixture, and (3) selection of best solvent for extraction. Solvents are selected from the list of registered compounds encountering more than 27,000 entries. Selection is made by best efficiency (depending on the task, solubility, selectivity, or distribution coefficient, etc.) and matching other requirements requested by the user. At user’s request, efficiency criteria are evaluated based on experimental data for binary mixtures or predictive models (UNIFAC variations).

Predictions can be compared to the available experimental data, and uncertainties are estimated for all efficiency criteria. Calculations of the properties of multi-component streams including composition at phase equilibria (flash calculations) are at the heart of process simulation engines. However, the accuracy of such calculations is generally unknown that often leads to overdesign of the operational units and results in significant additional cost. TDE provides a tool for the analysis of uncertainty of property calculations for multi-component streams. A process stream in TDE can be either a pure substance or mixture of chemical compounds under bubble, dew, or specified P-T conditions. VLE compositions and single-phase properties are calculated for process streams. Uncertainties are evaluated with the use of the covariance method where covariance matrices account for experimental uncertainties, curve deviations, and inadequacies of the models. Uncertainty analysis shows relative contributions to the total uncertainty from each component and pair of components.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, National Institute of Standards and Technology, Korea University
Optimal Design of Biodiesel Production Process from Waste Cooking Palm Oil

A design methodology for biodiesel production from waste cooking palm oil is proposed. The proposed method is flexible to the biodiesel process using various catalyst types: alkali and acid catalyst in homogenous and heterogeneous forms, and different process: enzyme process and supercritical process. A two-step approach of hydrolysis and esterification processes is also considered. Waste cooking palm oil consists of a mixture of triglyceride (e.g., trilaurin, tripalmitin, triolein, tristearin, trilinolein and trilinolenin) and free fatty acids (e.g., lauric acid, palmitic acid, stearic acid, oleic acid, linoleic and linolenic acid). A driving force approach and thermodynamic insight are employed to design separation units (e.g., flash separator and distillation) minimizing the energy consumption. Steady-state simulations of the developed biodiesel processes are performed and economic analysis is used to find a suitable biodiesel process. The results show that based on a net present value, the heterogeneous acid catalyzed process is the best process for biodiesel production. With the design methodology, the proposed biodiesel process can save the energy requirement of 41.5%, compared with a conventional process.

General information

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Chulalongkorn University
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Process design, biodiesel production, waste cooking palm oil, superstructure
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http://dtu.fic.cvts.dk/cgi-bin_fulltext_elsevier_pi_1877_7058_0042000c_12029281.pdf_key_368233681_rfr_id_info_sid_dlib.dtu.pdf
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Overcoming kinetic limitations in biocatalysis

General information
Overcoming kinetic limitations in biocatalysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Al-Haque, N. (Intern), Tufvesson, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2012
Event: Abstract from biocat 2012, Hamburg, Germany.
Main Research Area: Technical/natural sciences
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Phenomena-based Process Synthesis and Design to achieve Process Intensification

Process intensification (PI) has the potential to improve existing processes, necessary to achieve a more sustainable production. PI can be achieved at different levels. That is, the unit operations, functional and/or phenomena level. The highest impact is expected by looking at processes at the lowest level of aggregation: phenomena. Therefore, in this paper, a phenomena-based synthesis/design methodology is presented. Using this methodology, a systematic identification of necessary and desirable (integrated) phenomena as well as generation and screening of phenomena-based flowsheet options are made using a decomposition based solution approach. The developed methodology is highlighted through a case study involving the production of isopropyl-acetate.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Babi, D. K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Pages: 1697-1701
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Event: Poster session presented at biocat 2012, Hamburg, Germany.
Main Research Area: Technical/natural sciences
Publication: Research › Poster – Annual report year: 2012

Process Design and Evaluation for Chemicals Based on Renewable Resources

One of the key steps in process design is choosing between alternative technologies, especially for processes producing bulk and commodity chemicals. Recently, driven by the increasing oil prices and diminishing reserves, the production of bulk and commodity chemicals from renewable feedstocks has gained considerable interest. Renewable feedstocks usually cannot be converted into fuels and chemicals with existing process facilities due to the molecular functionality and
variety of the most common renewable feedstock (biomass). Therefore new types of catalytic methods as well as new types of processes for converting renewable feedstocks to bulk and commodity chemicals are required. In the future, it seems increasingly likely that a combination of biocatalysts (in the form of enzymes) as well as chemical catalysts will be needed in the production of bulk chemicals from renewable feedstocks. In addition, another characteristic of chemicals based on renewable feedstocks is that many alternative technologies and possible routes exist, resulting in many possible process flowsheets. The challenge for process engineers is then to choose between possible process routes and alternative technologies as well as to match different catalyst conditions. These kinds of problems are crucial, especially at the early stages of process development, when information is limited.

This thesis describes a methodological framework for dealing with the challenges and giving direction to research in the process development of chemicals based on renewable feedstocks. As an example, this thesis especially focuses on applying the methodology in process design and evaluation of the synthesis of 5-hydroxymethylfurfural (HMF) from the renewable feedstock glucose/fructose. The selected example is part of the chemoenzymatic process design of the synthesis 2,5-furandicarboxylic acid (FDA) from glucose.

By using the selected case study, the complexity and challenges for the process engineer to choose between different alternative routes and technologies as well as to combine two different kinds of catalysis (enzymatic catalysis and chemical catalysis) were illustrated.

Different process routes for the synthesis of HMF from fructose in the literature have been analyzed and evaluated. Using an aqueous route for HMF production is not economically feasible due to the low reaction yield. Using an anhydrous solvent for HMF synthesis is associated with high energy consumption and difficulties with solvent recycle in a large-scale production. The synthesis of HMF from fructose using a biphasic route is found to be promising, cost effective and give a better chance to be integrated with chemo-enzymatic cascades for producing FDA from glucose.

A process flowsheet using chemo-enzymatic cascades for HMF production from fructose has been proposed and evaluated. The process flowsheet is characterized by using glucose isomerase (EC 5.3.1.5) to convert glucose into fructose with a biphasic reaction for dehydration of fructose into HMF with recycle of the aqueous phase back to the enzymatic reaction. Costing analysis indicates the HMF production cost by the designed process is very sensitive to the dehydration reaction yield, the amount of solvent used in the whole process and the glucose price. In addition, increasing scale is also help to decrease the HMF production cost.

Using an ionic liquid (IL) route for HMF production has been evaluated with the dehydration reaction in [BMIm]Cl with different options starting from fructose and glucose with different initial concentrations. The HMF production cost is highly affected by the recycle of IL and catalyst.

Processes with a high feed concentration show better economic potential than processes with a low feed concentration. IL processes starting from fructose are more costly than IL processes starting from glucose. A high concentration feed of glucose showed the best economic potential.

To sum up, the dehydration reaction yield is found to be the key important factor to achieve a feasible production cost of HMF. The use of the organic solvent can not be avoided and plays a very important role in determining the process economics. Recycling (unconverted sugar, reaction medium and solvent) become essential issues for HMF processes to reach a feasible production cost. Future directions and suggestions for the synthesis of HMF from sugar in a large-scale have been proposed. The developed methodology is helpful in evaluation and giving research directions. The methodology can be applied to other chemical process design and evaluation problems and in particular those for the next generation of production processes.
Process Intensification of the Production of Di-Methyl Carbonate (DMC) Using a New Synthesis and Design Process Intensification Methodology Framework

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Technical University of Dortmund
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Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Paper 304a.pdf

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Oral presentation.
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Process Synthesis, Design and Intensification: An Integrated Approach

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Carnegie Mellon University, Federal University of Uberlândia
Authors: Babi, D. K. (Intern), Woodley, J. (Intern), Gani, R. (Intern), Siirola, J. J. (Ekstern), Rodrigues, F. (Ekstern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
AIChE_Paper 16b.pdf

Links:
https://aiche.confex.com/aiche/2012/webprogram/Paper265176.html

Bibliographical note
Plenary lecture.
Source: dtu
Source-ID: u::5311
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Process Systems Engineering, 1. Introduction
Production of Dialkyl Carbonates Via Reactive-Extractive and Pressure-Swing Distillations Using Unifac-CI VLE Model Predictions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, ChemProcess Technologies
Authors: Dada, E. A. (Ekstern), Mustaffa, A. A. (Intern), Gani, R. (Intern)
Publication date: 2012
Event: Abstract from 2012 AIChE Annual Meeting, Pittsburgh, PA, United States.
Main Research Area: Technical/natural sciences
Electronic versions: AIChE_Paper 324d.pdf

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Oral presentation.
Source: dtu
Source-ID: u::5318
Publication: Research - peer-review → Conference abstract for conference – Annual report year: 2012
Property Modelling and Databases in Product-Process Design

Properties of pure chemicals and their mixtures play an important role in the design of chemicals based products and the processes that manufacture them. Although, the use of experimental data in the design and/or analysis of these chemicals based products and their processes is desirable, they are not always available. Also, it may be too expensive or it may take too long to measure the required data. In these situations and when repetitive calculations are involved, as in process simulation, it is useful to have appropriate models to reliably predict the needed properties. For property model development, however, it is necessary to have a large database of measured property data that has been checked for consistency and accuracy.

The presentation will first introduce a database, in terms of its knowledge representation structure, the type and range of properties and chemical systems covered, and their internal consistency-accuracy checks. The database includes properties of organic chemicals, polymers and ionic liquids. There are also chemical class specific database sections, such as for solvents, aroma-chemicals, surfactants and emulsifiers. The use of this property database for model development will then be highlighted for a class of predictive models employing the group-contributionplus approach, where, the group-contribution (GC) method is combined with the atom-connectivity index (CI) method. Here, two parallel models are developed using the same dataset. However, during applications for property prediction, only the GC-model is used with the option to estimate missing group-contribution parameters through the CI-model. In this way, the application range of the GC-model is increased without the need for additional experimental data. This procedure for model development and use has been successfully employed for a range of pure component properties, polymer repeat-unit properties as well as mixture properties. For the mixture properties, liquid phase activity coefficients are modelled and then predicted through the UNIFAC-CI method. For bulk-properties of organic chemical mixtures, a GC-CI version of the PC-SAFT is used. The developed database and property prediction models have been combined into a properties-software that allows different product-process design related applications. The presentation will also briefly highlight applications of the software for virtual product-process design applications.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern), Sansonetti, S. (Intern)
Publication date: 2012
Event: Abstract from 18th Symposium on Thermophysical Properties, Boulder, CO, United States.
Main Research Area: Technical/natural sciences

Bibliographical note
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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
Authors: Abdul Samad, N. A. F. B. (Intern), Meisler, K. T. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Number of pages: 1
Publication date: 2012
Event: Abstract from APACT-12, Newcastle, United Kingdom.
Main Research Area: Technical/natural sciences
Electronic versions: NAS_APACT_12_Abstract_oral.pdf

Bibliographical note
Oral presentation
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Source-ID: u::4276
Publication: Research › Conference abstract for conference – Annual report year: 2012

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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CAPEC-PROCESS, Alfa Laval Copenhagen A/S
Authors: Hukkerikar, A. (Intern), Jones, M. N. (Intern), Sarup, B. (Ekstern), Abildskov, J. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 200-204
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Main Research Area: Technical/natural sciences
Process design, Sensitivity analysis, Uncertainty, Property prediction
Electronic versions: AMH_MJ_BS_JA_GSI_RaG_PSE2012_abstract.pdf
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Source-ID: u::4481
Publication: 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.

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Computer Aided Process Engineering Center
Authors: Jones, M. N. (Intern), Hukkerikar, A. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 18
Publication date: 2012
Event: Abstract from CHISA 2012, Prague, Czech Republic.
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Publication: Research › Conference abstract for conference – Annual report year: 2012

Separation of azeotropic mixtures
General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Technical University of Denmark
Authors: Fernández, E. (Ekstern), Gani, R. (Intern), Sin, G. (Intern)
Publication date: 2012
Event: Abstract from ANQUE ICCE 2012, Sevilla, Spain.
Main Research Area: Technical/natural sciences

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

Simultaneous design of ionic liquid entrainers and energy efficient azeotropic separation processes
A methodology and tool set for the simultaneous design of ionic liquid entrainers and azeotropic separation processes is presented. By adjusting the cation, anion, and alkyl chain length on the cation, the properties of the ionic liquid can be adjusted to design an entrainer for a given azeotropic mixture. Several group contribution property models available in literature have been used along with a newly developed group contribution solubility parameter model and UNIFAC model...
for ionic liquids (UNIFAC-IL). For a given azeotropic mixture, an ionic liquid is designed using a computer-aided molecular design (CAMD) method and the UNIFAC-IL model is used to screen design candidates based on minimum ionic liquid concentration needed to break the azeotrope. Once the ionic liquid has been designed, the extractive distillation column for the azeotropic mixture is designed using the driving force method with a new proposed feed stage scaling to minimize energy inputs. Along with the distillation column, an ionic liquid recovery stage is designed and simulations are used to determine the overall heat duty for the entire process for the best ionic liquid candidates. Use of a designed ionic liquid reduces material and energy requirements when compared to an ionic liquid known to experimentally break a given azeotrope but not designed using CAMD methods. The acetone–methanol and ethanol–water azeotropes are provided as examples.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, University of Kansas
Authors: Roughton, B. C. (Ekstern), Christian, B. (Ekstern), White, J. (Ekstern), Camarda, K. V. (Ekstern), Gani, R. (Intern)
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Publication date: 2012
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
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Web of Science (2013): Indexed yes
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Scopus rating (2009): SJR 1.154 SNIP 2.166
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Scopus rating (2008): SJR 1.293 SNIP 2.127
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Simultaneous Design of Ionic Liquids and CO2 Recovery Processes

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, University of Kansas
Authors: Chen, Q. (Ekstern), Christian, B. (Ekstern), Roughton, B. C. (Ekstern), Mitrofanov, I. (Intern), Camarda, K. C. (Ekstern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
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Links:
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Solventpro: The Solvent Selection and Design Framework

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mitrofanov, I. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
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Links:
https://aiche.confex.com/aiche/2012/webprogram/Paper271549.html

**Bibliographical note**
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

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Tsinghua University
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.004 SNIP 1.234 CiteScore 2.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Synthesis and Design of Processing Networks: Stochastic Formulation and Solution

In this contribution, we propose an integrated business and engineering framework for synthesis and design of processing networks under uncertainty. In our framework, an adapted formulation of the transhipment problem is integrated with a superstructure, leading to a Stochastic Mixed Integer Non Linear Program (sMINLP), which is solved to determine simultaneously the optimal strategic and tactical decisions with respect to the processing network, the material flows, raw material and product portfolio. The framework allows time-effective and robust formulation, solution and analysis of largescale synthesis problems in presence of uncertainty parameters, contributing to broaden the range of application of stochastic programming and optimization to real industrial problems. The framework is applied to an industrial case study based on soybean processing, to identify the optimal processing network under market and technical uncertainty.

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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Synthesis and Design of Processing Networks: Decision Making Under Uncertainty

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sin, G. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Publication date: 2012
Main Research Area: Technical/natural sciences

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Links:
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Oral presentation.
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Synthesis and design of processing networks: decision making under uncertainty and sensitivity analysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2012
Event: Abstract from CHISA 2012, Prague, Czech Republic.
Main Research Area: Technical/natural sciences

Electronic versions:
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Publication: Research › Conference abstract for conference – Annual report year: 2012

Synthesis and Design of Processing Networks: Stochastic Formulation and Solution

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Alfa Laval Copenhagen A/S
Authors: Quaglia, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences

Electronic versions:
AQ_Escape22_poster.pdf
Synthesis of Industrial Water Networks

Water is a valuable resource of great relevance for industrial activities. As water will become scarcer, optimization of its use is of key importance. The issue of water allocation and reuse through mathematical optimization has been addressed in various literature works [1, 2]. However most of the water networks proposed comprise few contaminants and do not consider critical parameters for wastewater treatment equipment, such as limiting inlet concentrations, flow rates, and other specific design constraints. Thus, these networks are arguably not fit to manage the complexity of a real industrial case (in terms of number of contaminants, number of processing options, design constraints etc.).

In this work, a systematic framework for the formulation and solution of water networks problems is proposed, based on the modification of an earlier work [3]. The optimization problem is formulated as a Mixed Integer Non Linear Programming (MINLP), which is solved to identify the best wastewater treatment process among a set of predefined alternatives, according to selected optimum criteria. The optimum criteria may be minimum operating, capital, or total cost, freshwater consumption, treated water discharge and/or concentration of a selected contaminant. The final design can then be refined through a more detailed model with any appropriate process simulator. The methodology employed is as follows. First, the sources of wastewater and treatment objectives need to be identified. A superstructure of available technologies is used in order to identify process alternatives. The superstructure is built dividing the treatment operation in tasks to remove the various pollutants and considering process units currently used in industry. Then, the objective function is chosen and the problem is formulated as a MINLP optimization problem, which is solved in GAMS.

In order to demonstrate and highlight the features of the tool, a case study dealing with refinery wastewater purification is presented. A superstructure containing technological alternatives for water purification is built, and the optimization problem is formulated and solved for different scenarios.

With respect to the superstructures presented in literature, the one developed here accommodates a more detailed modeling of the water treatment units and a wider range of contaminants. This makes it flexible for various applications and can be used to provide guideline for the process design of the treatment of different types of wastewater sources. This approach constitutes a useful and flexible tool to design wastewater treatment systems for new plant or retrofit or expansion of existing plants. The tool also allows for the evaluation of the effect of different scenarios e.g. different optimum criteria, wastewater sources, environmental regulations on water discharge, contaminant loads on purified water to recycle etc.

Bibliographical note

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Systematic identification of crystallization kinetics within a generic modelling framework

A systematic development of constitutive models within a generic modelling framework has been developed for use in design, analysis and simulation of crystallization operations. The framework contains a tool for model identification.
connected with a generic crystallizer modelling tool-box, a tool for data handling and translation as well as model application features. Through this framework it is possible, for a wide range of crystallization processes, to generate the necessary problem-system specific models; to identify the parameters for constitutive models; and to handle or translate raw crystallization data. Application of the systematic framework is highlighted through a sucrose crystallization case study, for which the parameters for nucleation and crystal growth are first estimated from the available measured data and are then applied to study the crystallization operation.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Abdul Samad, N. A. F. B. (Intern), Meisler, K. T. (Intern), Gernaey, K. (Intern), von Solms, N. (Intern), Gani, R. (Intern)
Pages: 945-949
Publication date: 2012

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Main Research Area: Technical/natural sciences

**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.

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ThermoData Engine: Extension to Solvent Design and Multi-component Process Stream Property Calculations with Uncertainty Analysis

ThermoData Engine (TDE, NIST Standard Reference Databases 103a and 103b) is the first product that implements the concept of Dynamic Data Evaluation in the fields of thermophysics and thermochemistry, which includes maintaining the comprehensive and up-to-date database of experimentally measured property values and expert system for data analysis and generation of recommended property values at the specified conditions along with uncertainties on demand. The most recent extension of TDE covers solvent design and multi-component process stream property calculations with uncertainty analysis.

Solvent Design function serves three tasks: (1) selection of best solvent for a solid solute, (2) search for a selective solvent for a solid binary mixture, and (3) selection of best solvent for extraction. Solvents are selected from the list of registered compounds encountering more than 27,000 entries. Selection is made by best efficiency (depending on the task, solubility, selectivity, or distribution coefficient, etc.) and matching other requirements requested by the user. At user’s request, efficiency criteria are evaluated based on experimental data for binary mixtures or predictive models (UNIFAC variations). Predictions can be compared to the available experimental data, and uncertainties are estimated for all efficiency criteria. Calculations of the properties of multi-component streams including composition at phase equilibria (flash calculations) are at the heart of process simulation engines. However, the accuracy of such calculations are generally unknown that often leads to overdesign of the operational units and results in significant additional cost. TDE provides a tool for the analysis of uncertainty of property calculations for multi-component streams. A process stream in TDE can be either a pure substance or mixture of chemical compounds under bubble, dew, or specified P-T conditions. VLE compositions and single-phase properties are calculated for process streams. Uncertainties are evaluated with the use of the covariance method where
covariance matrices account for experimental uncertainties, curve deviations, and inadequacies of the models. Uncertainty analysis shows relative contributions to the total uncertainty from each component and pair of components.

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.

A model-based framework for design of intensified enzyme-based processes

This thesis presents a generic and systematic model-based framework to design intensified enzyme-based processes. The development of the presented methodology was motivated by the needs of the bio-based industry for a more systematic approach to achieve intensification in its production plants without an excessive investment in experimental resources. Process intensification has recently gained a lot of attention since it is a holistic approach to design safer, cleaner, smaller, cheaper and more efficient processes. This dissertation proposes a methodological approach to achieve
intensification in enzyme-based processes which have found significant application in the pharmaceutical, food, and renewable fuels sector. The framework uses model-based strategies for (bio)-chemical process design and optimization, including the use of a superstructure to generate all potential reaction(s)-separation(s) options according to a desired performance criteria and a generic mathematical model represented by the superstructure to derive the specific models corresponding to a specific process option. In principle, three methods of intensification of bioprocess are considered in this thesis: 1. enzymatic one-pot synthesis, where, for example, the combination of two enzymatic reactions in one single reactor is examined; 2. chemo-enzymatic one pot synthesis, where, for example, one enzymatic reaction and one alkaline catalytic reaction occur simultaneously in a single reactor; and 3. in-situ product recovery/removal (ISPR), where, for example, a separation step is integrated with the reaction step. Often, enzyme-based processes have limited productivity and yield, which may be due to the unfavorable reaction equilibrium, product inhibition to the enzyme and/or product degradation. Additionally, downstream processing for enzyme-based processes is difficult and a way to simplify it is by reducing the reaction and separation steps by for example, combining the reaction and separation in a single processing step. The implementation of intensification methods usually involves experiment-based investigation which causes limitations in the search space of process options leading to a high risk of implementing sub-optimal processes. Therefore, applying the framework presented in this thesis, all possible process options can be considered, and using a hierarchical decomposition approach for optimization, the search space is reduced to locate the candidate process options, giving an optimal design where further experimental efforts can be focused on. The application of a generic and systematic model-based framework is illustrated through a case study involving the production of an important intermediate pharmaceutical: N-acetyl-D-neuraminic acid (Neu5Ac). A second case study is added and deals with the enzymatic production of biodiesel.

Computer-Aided Modeling of Lipid Processing Technology

Vegetable oils and fats have an important role in human nutrition and in the chemical industry since they are a source of energy, fat-soluble vitamins, and now also in the production of renewable sources of energy. Nowadays as the consumer preferences for natural products and healthier foods increase along with growing interest in biofuels, the oleochemical industry faces in the upcoming years major challenges in terms of design and development of better products and more sustainable processes to make them. Computer-aided methods and tools for process synthesis, modeling and simulation are widely used for design, analysis, and optimization of processes in the chemical and petrochemical industries. These computer-aided tools have helped the chemical industry to evolve beyond commodities toward specialty chemicals and ‘consumer oriented chemicals based products’. Unfortunately this is not the case for the edible oil and biodiesel industries. The oleochemical industry lags behind the chemical industry in terms of thermophysical property modeling and development of computational tools suitable for the design/analysis, and optimization of lipid-related processes. The aim of this work has been to develop systematic computer-aided methods (property models) and tools (database) related to the prediction of the necessary physical properties suitable for design and analysis of processes employing lipid technologies. The methods and tools include: the development of a lipid-database (CAPEC_Lipids_Database) of collected experimental data from the open literature, data from industry, and, generated data from validated predictive property models; as well as the development of a database user-interface and an external version of this database, for use in commercial process simulators, for fast adoption-analysis of property prediction models and for fast development of process models not available in process simulators. This was achieved by first identifying and classifying the lipid compounds found in the edible oil and biodiesel industries. Then creating a list of the thermophysical properties needed for model-based design and analysis of edible oil and biodiesel processes. Next, collection of the available experimental data from different sources for the identified lipid compounds. Finally, selecting and adopting the appropriate models to predict the necessary properties, to fill-out the lipid-database and to make it suitable for application with other computer-aided tools (such as commercial process simulators). The developed computer-aided methods (property models) and tools (CAPEC_Lipids_Database) have been linked to the proposed methodology for the design/analysis of lipid-related processes. In this PhD thesis the analysis, in terms of their design variables and their impact in the process behavior, of three lipid-related processes has been performed: the solvent recovery section of the extraction of crude soybean oil, the deodorization of palm oil, and the deacidification of soybean oil.
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 four sequential hierarchical sub-problems: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, and (iv) final selection and verification. Using thermodynamic and process insights, a bounded search space is first identified. This feasible solution space is further reduced to satisfy the process design and controller design constraints in sub-problems 2 and 3, respectively, until in the final sub-problem all feasible candidates are ordered according to the defined performance criteria (objective function). The final selected design is then verified through rigorous simulation. In the pre-analysis sub-problem, the concepts of attainable region and driving force are used to locate the optimal process-controller design solution in terms of optimal condition of operation from design and control viewpoints. The targets for the design-control solution are defined at the maximum point of the attainable region and driving force diagrams. Defining the targets at the maximum point of the attainable region and driving force diagram ensure the optimal solution not only for the process design but also for the controller design. From a process design point of view at these targets, the optimal design objectives can be obtained. Then by using the reverse solution approach, values of design-process variables that match those targets are calculated in Stage 2. Using model analysis, controllability issues are incorporated in Stage 3 to calculate the process sensitivity and to pair the identified manipulated variables with the corresponding controlled variables. From a controller design point of view, at targets defined in Stage 1, the sensitivity of controlled variables with respect to disturbances is at the minimum and the sensitivity of controlled variables with respect to manipulated variables is at the maximum. Minimum sensitivity with respect to disturbances means that the controlled variables are less sensitive to the effect of disturbances and maximum sensitivity with respect to manipulated variables determines the best controller structure. Since the optimization deals with multicriteria objective functions, therefore, in Stage 4, the objective function is calculated to verify the best (optimal) solution that satisfies design, control and economic criteria. From an optimization point of view, solution targets at the maximum point of the attainable region and driving force diagrams are shown the higher value of the objective function, hence the optimal solution for the IPDC problem is verified. While other optimization methods may or may not be able to find the optimal solution, depending on the performance of their search algorithms and computational demand, this method using the attainable region and driving force concepts is simple and able to find at least near-optimal designs (if not optimal) to IPDC problems. The developed methodology has been implemented into a systematic computer-aided framework to develop a software called ICAS-IPDC. The purpose of the software is to support engineers in solving process design and controller design problems in a systematic and efficient way. The proposed methodology has been tested using a series of case studies that represents three different systems in chemical processes: a single reactor system, a single separator system and a reactor-separator-recycle system.
Achieving Process Intensification: A Phenomena-Based Synthesis/Design Methodology

General information
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A Combined Heuristic and Indicator-based Methodology for Design of Sustainable Chemical Process Plants
The current emphasis on sustainable production has prompted chemical plants to minimize raw material and energy usage without compromising on economics. While computer tools are available to assist in sustainability assessment, their applications are constrained to a specific domain of the design synthesis problem. This paper outlines a design synthesis strategy that integrates two computer methodologies – ENVOPEXpert and SustainPro – for simultaneous generation, analysis, evaluation, and optimization of sustainable process alternatives. ENVOPEXpert diagnoses waste sources, identifies alternatives, and highlights trade-offs between environmental and economic objectives. This is complemented by SustainPro which evaluates the alternatives and screens them in-depth through indicators for profit and energy, water, and raw material usage. This results in accurate identification of the root causes, comprehensive generation of design alternatives, and effective reduction of the optimization search space. The frame-work is illustrated using an acetone process and a methanol and dimethyl ether production case study.

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A framework for API solubility modelling

The solubility of solid organic compounds in water and organic solvents is a fundamental thermodynamic property for many purposes such as product-process design and optimization, for the chemical and pharmaceutical industry. Experimental literature solubility data are usually scarce and temperature-dependent measurements are expensive in terms of time and resources. The few available data are badly organized and difficult to use for fast solubility calculations and solvent screening. Available models often require time consuming and complex implementation together with a good user expertise for their efficient use. In addition, most of the models are not predictive and requires experimental data for the calculation of the needed parameters. This work aims at developing an efficient framework for the solubility modelling of Active Pharmaceutical Ingredients (API) in water and organic solvents. With this framework, the user will be able to solve a specific design/verification problem, quickly and simply with no expert knowledge. At first, a solubility database containing solid-liquid equilibrium data is developed. Then, available and validated models for the calculation of solid-liquid equilibrium (NRTL-SAC, PC-SAFT) are used for solubility calculations when the needed interaction parameters or
experimental data are available. The CI-UNIFAC is instead used when the previous models lack interaction parameters or when solubility data are not available. A new GC+ model for APIs solvent selection based on the hydrophobicity, hydrophilicity and polarity information of the API and solvent is also developed, for performing fast solvent selection and screening. Eventually, all the previous developments are integrated in a framework for their efficient and integrated use. Two case studies are presented: the first highlights the solubility modelling tool for the calculation of APIs solubility in lipids with the PC-SAFT equation of state; the second highlights the solvent selection tool for the identification of feasible solvents for nitro-APIs.

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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 N<10>. Permeance analysis revealed poresizes (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).

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Analysis and Application of GC Plus Models for Property Prediction of Organic Chemical Systems

In this paper, a detailed analysis of the performance and trends of predictions of vapour–liquid phase equilibrium with the UNIFAC-CI model, employing a method to predict missing group interaction parameters (GIPs) through the use of connectivity indices, are presented. The cases where the model using the predicted GIPs perform well and cases where the performance is unreliable are investigated. The causes for the unreliable performance of the UNIFAC-CI model are explained and results from one of the remedies that gave very good results are presented. The extrapolation features of the UNIFAC-CI model with the predicted GIPs in solid–liquid phase equilibria calculations involving precipitation of organic chemicals are also presented. Finally, the application of the GCPlus approach to reference modified UNIFAC (Dortmund) model is presented in terms of new and extended parameter tables.

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An Innovative Synthesis Methodology for Process Intensification

Process intensification (PI) has the potential to improve existing processes or create new process options, which are needed in order to produce products using more sustainable methods. A variety of intensified equipment has been developed which potentially creates a large number of options to improve a process. However, to date only a limited number have achieved implementation in industry, such as reactive distillation, dividing wall columns and reverse flow reactors. A reason for this is that the identification of the best PI option is neither simple nor systematic. That is to decide where and how the process should be intensified for the biggest improvement. Until now, most PI has been selected based on case-based trial-and-error procedures, not comparing different PI options on a quantitative basis.

Therefore, the objective of this PhD project is to develop a systematic synthesis/design methodology to achieve PI. It allows the quick identification of the best PI option on a quantitative basis and will push the implementation and acceptance of PI in industry. Such a methodology should be able to handle a large number of options. The method of solution should be efficient, robust and reliable using a well-defined screening procedure. It should be able to use already existing PI equipment as well as to generate novel PI equipment.

This PhD-project succeeded in developing such a synthesis/design methodology. In order to manage the complexities involved, the methodology employs a decomposition-based solution approach. Starting from an analysis of existing processes, the methodology generates a set of PI process options. Subsequently, the initial search space is reduced through an ordered sequence of steps. As the search space decreases, more process details are added, increasing the complexity of the mathematical problem but decreasing its size. The best PI options are ordered in terms of a performance index and a related set are verified through detailed process simulation. Two building blocks can be used for the synthesis/design which is PI unit-operations as well as phenomena. The use of PI unit-operations as building block aims to allow a quicker implementation/retrofit of processes while phenomena as building blocks enable the ability to develop novel process solutions beyond those currently in existence. Implementation of this methodology requires the use of a number of methods/algorithms, models, databases, etc., in the different steps which have been developed. PI unit-operations are stored and retrieved from a knowledge-base tool. Phenomena are stored and retrieved from a phenomena library.

The PI synthesis/design methodology has been tested for both building blocks on a number of case studies from different areas such as conventional and bio-based bulk chemicals as well as pharmaceuticals.
Application of a Synthesis and Design Methodology to achieve Process Intensification

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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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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 fulfill 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 features like variable classification, degree of freedom analysis, incidence matrix generation, optimal equation ordering, eigenvalue analysis. Once the models have been constructed and analysed the modelling framework incorporates 3 application work-flows for: 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.

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A retrofit strategy to achieve "Fast, Flexible, Future (F3)" pharmaceutical production processes

In the work reported here, a substrates adoption methodology for a series of similar substrates has been developed as part of a retrofit strategy. The objective is to achieve "fast, flexible and future" pharmaceutical production processes by adapting a generic modular process-plant template. Application of the methodology is illustrated through a case study from the pharmaceutical industry. Use of computer-aided models, methods and tools as part of the methodology is also highlighted.

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A retrofit strategy to achieve "Fast, Flexible, Future (F3)" pharmaceutical production processes
A systematic framework for CAFD and resources allocation optimisation using MINLP in vegetable oil processing

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 Synthesis 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.

A systematic methodology for the design of continuous active pharmaceutical ingredient production processes

Continuous pharmaceutical manufacturing (CPM) has emerged as a powerful technology to obtain higher reaction yields and improved separation efficiencies, potentially leading to simplified process flowsheets, reduced total costs, lower environmental impacts, and safer and more flexible production. However, the change from batch-wise production towards continuous operation and the definition of flexible design spaces requires a high degree of process knowledge. Process Systems Engineering (PSE) offers multiple methods and tools which can assist in efficient knowledge acquisition, structuring and representation, as well as how to employ this knowledge for process (re-)design. The aim of this paper is to introduce a methodology that systematically identifies already existing PSE methods and tools which can assist in the design of CPM processes. This methodology has been applied to a process for the production of an API developed by H. Lundbeck A/S, demonstrating the mentioned potential benefits that CPM can offer.
A systematic methodology for the design of continuous active pharmaceutical ingredient production processes

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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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A systematic synthesis and design methodology to achieve process intensification in (bio)chemical processes

Process intensification (PI) has the potential to improve existing processes or create new process options which are needed in order to produce products using more sustainable methods. Potentially, PI creates an enormous number of process options. For identification where and how the process should be intensified for biggest improvement, process synthesis and design tools are applied which results in the development of a systematic methodology incorporating PI. In order to manage the complexity of PI process options in which a feasible and optimal process solution may exist, the solution procedure of this methodology is based on the decomposition approach. Starting from an analysis of existing processes, this methodology generates a set of feasible process options and reduces their number through several screening steps until from the remaining feasible options, the optimal is found. In this presentation, the application of the computer-aided systematic synthesis and design methodology is highlighted via a case study which is the chemo-enzymatic synthesis of N-acetyl-D-neuraminic acid (Neu5Ac)).

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.
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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Chemical-Based Formulation Design: Virtual Experimentation
This paper presents a software, the virtual Product-Process Design laboratory (virtual PPD-lab) and the virtual experimental scenarios for design/verification of consumer oriented liquid formulated products where the software can be used. For example, the software can be employed for the design of the active ingredient-solvent mixture and/or their verification in terms of the product function. These consumer products are still primarily designed, developed and/or tested
through experiment-based trial and error approaches. However, using the powerful methodologies and tools developed within the process system engineering community, it is possible now to replace, at least, some of the experimental steps with efficient and validated model-based approaches. For example, the search space can be significantly reduced through computer-aided screenings of the active ingredient (AI), the solvent mixture, the additives and/or their mixtures (formulations). Therefore, the experimental resources can focus on a few candidate product formulations to find the best product. The virtual PPD-lab allows various options for experimentations related to design and/or verification of the product. For example, the selection and verification of the functions of the AI; the design of solvent mixtures for the delivery of the AI; the stability test of the liquid formulated product; the selection of additives such as aroma compounds to be added to the products to enhance their quality; the generation of a list of candidate formulations; the addition of the missing chemicals to an incomplete formulation and the verification of the final product. The software is based on a framework that allows quick implementation of different design/verification work-flows and their associated models, methods, tools and data. The software contains a suite of databases with data of AIs used in different products (such as insect repellents), solvents classified in terms of special characteristics (such as solubility in water), and additives classified in terms of their application (such as aroma agents, wetting agents and preservatives). In addition, the software has built-in intelligence through implemented knowledge-bases related to transforming product attributes (consumer needs) to a set of physical-chemical properties; templates (work-flows) for specific product types are also available; guidance for property model (such as pure component properties and mixture properties) selection and adaptation is provided; the selection and use of models for product verification is also possible (such as stability of liquid and evaporation of the solvent after application of the product). Finally, the software has a collection of algorithms (such as CAMD, mixture design, model adaptation). All of the above helps to perform virtual experiments by blending chemicals together and observing their predicted behaviour. The paper will highlight the application of the virtual PPD-lab in the design and/or verification of different consumer products (paint formulation, hair spray, sunscreen lotion, insect repellent lotion). The results of the virtual experimentations will be illustrated through the (initial) base case designs that were obtained and their verification through real experiments and/or available product data analysis.

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**Chemical Engineering Education - Current and Future Trends**

The chemical engineering industry today is changed from the chemical industry of twenty-five years ago. Clear evidence of this change comes from the jobs taken by graduating chemical professionals in North America, Europe, and some of the Asian countries. Twenty-five years ago, eighty percent of these graduating students went to the commodity chemical industry, exemplified by Dupont, Exxon, Shell, ICI, BASF and Dow, to name a few. Now, twenty percent do. Twenty-five years ago, around ten percent went to product-oriented businesses like PPG, Pfizer, and 3M. Now, fifty percent do. The chemical industry now has a product focus. With this shift of the chemical industry, what should be the curriculum of the chemical engineering degrees at the BSc- and MSc-levels, and, are the skill set of chemical engineers appropriate for this altered chemical industry? While the basic skill set, defined by the core topics (transport phenomena, separations, reaction engineering, etc.) must remain strong, should the applications that currently emphasize commodity chemicals also include new topics such as sustainability, and product design? In Europe, the European Federation of Chemical Engineering (EFCE) has taken a leading role to define the chemical engineering curriculum. The result has been a set of recommendations for the first (BSc), second (MSc) and third (PhD) cycle chemical engineering education aligned to the Bologna Process. They recommend that students studying towards bachelor and masters qualifications should be measured on their level of knowledge and the understanding they develop, rather than the amount of time they spend with the tutors. According to the Bologna Process, the first and the second cycle degrees should have different orientations and various profiles in order to accommodate a diversity of individual, academic and labour-market needs. Within Europe, two types of higher education in chemical engineering can be found: more research-oriented or more application-oriented first cycle programmes. Both types of studies cover a period of 3-4 academic years and 60 credits per year. After completion of the first cycle, students can continue their study with a second cycle program of chemical engineering with 90-120 credits for a further 18-24 months. For the first and second cycles, the EFCE recommend a set of programme outcomes (knowledge and understanding, engineering analysis, engineering design, investigations, engineering practice and transferable skills) and a set guidelines (core curriculum, teaching and learning, industrial experience, review of the education process and student assessment) to achieve them, with special emphasis to the ability to solve problems. They also propose a minimum set of subjects required to define a course as chemical engineering and the level of achievement that might reasonably be expected at different levels. The talk will give an overview of the recommendations of the EFCE and highlight their implementation at the Technical University of Denmark’s chemical engineering programmes. Also,
some of the issues related to the changing needs of the chemical industry will be discussed.

**Chemical Engineering Education in a Bologna Three Cycle Degree System**

For the purpose of harmonization of European higher education, Europe’s education system has been going through major changes under what is commonly known as the "Bologna Process". The Bologna declaration in 1999 was the start of the introduction of a three cycle degree system in higher education in Europe. To date, many European universities have adopted this degree structure. The Working Party on Education (WPE) of the European Federation of Chemical Engineering (EFCE) carried out research to determine the contents of higher education in chemical engineering (ChE) and related disciplines such as applied chemistry and process engineering throughout Europe. The result has been a set of recommendations for the first (BS), second (MS) and third (PhD) cycle chemical engineering education aligned to the Bologna Process. They recommend that students studying towards bachelor and masters qualifications should be measured on their level of knowledge and the understanding they develop, rather than the amount of time they spend with the tutors. The recommendations also suggest that students studying for a PhD or doctorate degree should be encouraged to further develop their abilities to manage independent research work. The importance of learning outcomes has been emphasized at all levels. According to the Bologna Process, the first and the second cycle degrees should have different orientations and various profiles in order to accommodate a diversity of individual, academic and labour-market needs. Within Europe, two types of higher education in ChE can be found: more research-oriented or more application-oriented first cycle (bachelor) programmes. Both types of studies cover a period of 3-4 academic years and 60 credits per year. After completion of the first cycle, students can continue their study with a second cycle program of ChE with 90-120 credits for a further 18-24 months. For the first and second cycles, the WPE of the EFCE adopt the European Accreditation of Engineering Programmes (EUR-ACE) framework and recommend a set of programme outcomes (knowledge and understanding, engineering analysis, engineering design, investigations, engineering practice and transferable skills) and a set guidelines (core curriculum, teaching and learning, industrial experience, review of the education process and student assessment) to achieve them. They also propose a minimum set of subjects required to define a course as chemical engineering and the level of achievement that might reasonably be expected at different levels. The talk will give an overview of the recommendations of the WPE and highlight their implementation at the Technical University of Denmark’s ChE programmes, whose accreditation has been approved by the EUR-ACE. Courses on process and product design will be used as examples.

**Chemicals-Based Formulation Design: Virtual Experimentations**

This paper presents a systematic procedure for virtual experimentations related to the design of liquid formulated products. All the experiments that need to be performed when designing a liquid formulated product (lotion), such as ingredients selection and testing, solubility tests, property measurements, can now be performed through the virtual Product-Process Design laboratory [1], [2] and [3]. The user can mimic different experimental scenarios (different products and specifications) and obtain a base case product which could then be tested and amended through real experiments. A case study on the design of an insect repellent lotion will show that the software is an essential instrument.
in decision making, and that it reduces time and resources since experimental efforts can be focused on one or few product alternatives.

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**Computer Aided Flowsheet Design using Group Contribution Methods**
In this paper, a systematic group contribution based framework is presented for synthesis of process flowsheets from a given set of input and output specifications. Analogous to the group contribution methods developed for molecular design, the framework employs process groups to represent different unit operations in the system. Feasible flowsheet configurations are generated using efficient combinatorial algorithms and the performance of each candidate flowsheet is evaluated using a set of flowsheet properties. A systematic notation system called SFILES is used to store the structural information of each flowsheet to minimize the computational load and information storage. The design variables for the selected flowsheet(s) are identified through a reverse simulation approach and are used as initial estimates for rigorous simulation to verify the feasibility and performance of the design.

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simulation to verify the feasibility and performance of the design.

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

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 an 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 computeraided modelling framework and the developed software
tool.
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.
Computer-Aided Modelling Methods and Tools

The development of models for a range of applications requires methods and tools. In many cases a reference model is required that allows the generation of application specific models that are fit for purpose. There are a range of computer aided modelling tools available that help to define the model, generate the model and provide a range of toolboxes to aid model analysis, solution and results generation. This chapter describes the basic model structures that commence with a definition of the balance volumes and then discuss the conservation equations, constraints and constitutive equations. To illustrate these concepts a number of examples are used. These include models of polymer membranes, distillation and catalyst behaviour. Some detailed considerations within these models are stated and discussed. Model generation concepts are introduced and ideas of a reference model are given that shows a taxonomy of aspects around conservation, constraints and constitutive relations. Aspects of the ICAS-MoT toolbox are given to illustrate the functionality of a computer aided modelling tool, which incorporates an interface to MS Excel.
Computer Aided Modelling – Opportunities and Challenges
This chapter considers the opportunities that are present in developing, extending and applying aspects of computer-aided modelling principles and practice. What are the best tasks to be done by modellers and what needs the application of CAPE tools? How do we efficiently develop model-based solutions to significant problems? The important issues of workflow and data flow are discussed together with fit-for-purpose model development. As well, the lack of tools around multiscale modelling provides opportunities for the development of efficient tools to address such challenges. The ability to easily generate new models from underlying phenomena continues to be a challenge, especially in the face of time and cost constraints. Integrated frameworks that allow flexibility of model development and access to a range of embedded tools are central to future model developments. The challenges and opportunities are discussed for such systems.

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 the 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] 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 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. 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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 the 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] 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 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 the 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] 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 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.
Computers & Chemical Engineering: Best paper of 2009
The Editorial Advisory Board of the Journal has assessed the papers published in Volume 33 by means of a three stage process of nomination and balloting. We are pleased to announce that the 2009 Best Paper of the Year Award goes to J.M. Harrold and R.S. Parker for their paper entitled “Clinically relevant cancer chemotherapy dose scheduling via mixed-integer optimization” (Vol. 33, Issue 12, 2042–2054, 2009). Our hearty congratulations to the co-authors!

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Purdue University
Authors: Venkatasubramanian, V. (Ekstern), Gani, R. (Intern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Constitutive Models

This chapter presents various types of constitutive models and their applications. There are 3 aspects dealt with in this chapter, namely: creation and solution of property models, the application of parameter estimation and finally application examples of constitutive models. A systematic procedure is introduced for the analysis and solution of property models. Models that capture and represent the temperature dependent behaviour of physical properties are introduced, as well as equation of state models (EOS) such as the SRK EOS. Modelling of liquid phase activity coefficients are also covered, illustrating several models such as the Wilson equation and NRTL equation, along with their solution strategies. A section shows how to use experimental data to regress the property model parameters using a least squares approach. A full model analysis is applied in each example that discusses the degrees of freedom, dependent and independent variables and solution strategy. Vapour-liquid and solid-liquid equilibrium is covered, and applications to droplet evaporation and kinetic models are given.

General information

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Universidad Autonoma Metropolitana, University of Queensland
Authors: Sales-Cruz, M. (Ekstern), Piccolo, C. (Intern), Heitzig, M. (Intern), Cameron, I. (Ekstern), Gani, R. (Intern)
Number of pages: 557
Pages: 87-124
Publication date: 2011

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Volume: 5
Publisher: Elsevier Science
Editors: Cameron, I., Gani, R.
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Physical properties, Vapour Liquid Equilibrium, Property models, SRK equation of state, Solid Liquid Equilibrium, Parameter estimation, NRTL equation of state, Constitutive equations
Source: orbit
Source-ID: 283363
Publication: Research - peer-review › Book chapter – Annual report year: 2011

Design and analysis of membrane based process intensification and hybrid processing options
Design of an Optimal Biorefinery

In this paper we propose a biorefinery optimization model that can be used to find the optimal processing route for the production of ethanol, butanol, succinic acid and blends of these chemicals with fossil fuel based gasoline. The approach unites transshipment models with a superstructure, resulting in a Mixed Integer Non-Linear Program (MINLP). We consider a specific problem based on a network of 72 processing steps (including different pretreatment steps, hydrolysis, fermentation, different separations and fuel blending steps) that can be used to process two different types of feedstock. Numerical results are presented for four different optimization objectives (maximize yield, minimize costs, minimize waste and minimum fixed cost), while evaluating different cases (single product and multi-product).
Design of formulated products: a systematic methodology

In chemical product design one tries to find a product which exhibits the desired (target) behavior specified a priori. The identity of the ingredients of chemical-based products maybe unknown at the start, but some of their desired qualities and functions are usually known. A systematic model-based computer-aided methodology for design and verification of a class of chemical-based products (liquid formulations) is presented. This methodology is part of an integrated three-stage approach for design/verification of liquid formulations where stage-1 generates a list of feasible product candidates and/or verifies a specified set through a sequence of predefined activities (work-flow). Stage-2 and stage-3 (not presented here) deal with the planning and execution of experiments, for product validation. Four case studies have been developed to test the methodology. The computer-aided design (stage-1) of a paint formulation and an insect repellent lotion are presented.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Hong Kong University of Science and Technology
Authors: Conte, E. (Intern), Gani, R. (Intern), Ng, K. (Ekstern)
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.004 SNIP 1.234 CiteScore 2.31
Design of tailor-made chemical blend using a decomposition-based computer-aided approach

Computer aided techniques form an efficient approach to solve chemical product design problems such as the design of blended liquid products (chemical blending). In chemical blending, one tries to find the best candidate, which satisfies the product targets defined in terms of desired product attributes (properties). The systematic computer-aided technique first establishes the search space, and then narrows it down in subsequent steps until a small number of feasible and promising candidates remain. At this point, experimental work may be conducted to verify if any or all the candidates satisfy the desired product attributes. Alternatively, rigorous modeling could also be used in this final step. In other words, the candidates are quickly generated and screened until a small number is left for final selection and evaluation by experiments and/or rigorous modeling. This paper presents a design methodology for blended liquid products that identifies a set of feasible chemical blends. The blend design problem is formulated as a Mixed Integer Nonlinear Programming (MINLP) model where the objective is to find the optimal blended gasoline or diesel product subject to types of chemicals and their compositions and a set of desired target properties of the blended product as design constraints. This blend design problem is solved using a decomposition approach, which eliminates infeasible and/or redundant candidates gradually through a hierarchy of (property) model based constraints. This decomposition method reduces the search space in a systematic manner and the general blend design problem is decomposed into two stages. The first stage investigates the mixture stability where all unstable mixtures are eliminated and the stable blend candidates are retained for further testing (note that all blends must be stable liquid mixture). In the second stage, the blend candidates have to satisfy a set of target properties that are ranked according to a specified priority. Finally, a short list of candidates, ordered in terms of specified performance criteria, is produced for final testing and selection. The application of this systematic and computer-aided approach is illustrated through a case study involving the design of blends of gasoline with oxygenated compounds resulting from degradation and fermentation of biomass for use in internal combustion engines. Emphasis is given here on the concepts used and on the validation of the property models, mainly, the Reid vapor
Development of a fast and flexible generic process for the reduction of nitro compounds

The hydrogenation of aromatic nitro substrates is a frequently used reaction in the multi-step fabrication of active pharmaceutical ingredients (APIs). Today most pharmaceutical production processes are performed in batch mode. In the frame of the C2-campaign speed is an important factor during the production of a multitude of possible API's. A generic reactor set-up able to be adapted for the transformation of a specific substrate would reduce the development time and thereby the campaign time significantly. In the frame of the EU-project F3-Factory such a flexible and continuous reaction system for this important reaction class able to produce 1-5 kg API is being developed. To allow for an easy and fast

Design of Tailor-made Fuel Blends of Gasoline and Bio-fuels

Development and Analysis of Original UNIFAC-CI and Modified (Dortmund) UNIFAC-CI Models for Predictions of VLE and SLE Systems
adaptation of this process for a range of nitro substrates a substrates adoption methodology (SAM) is also being developed. A literature study of the nature of different reduction methods (H2 gas, H-Donor, CO gas, etc.) led to the conclusion that the liquid phase reduction of aromatic nitro substrates by either hydrogen gas or an H-donor is the most selective method. Following the requirements of that reaction type a flexible and modular reactor for the liquid phase reduction with a heterogeneous slurry catalyst was designed that can be adapted for reduction of a range of nitro compounds. The generic process provides the possibilities of swapping out a reactor or work up technology as required. The equipments of the generic process should be also able to operate at wider range of operational variables making it suitable for a range of substrates. The SAM identifies the necessary changes to a generic process and plant in order to adapt it for a given substrate. The objectives of this presentation is to highlight the design of a generic nitro reduction process and to demonstrate the application of this generic process on a pharmaceutical manufacturing case study involving the nitro reduction of 6-Nitroquinoline.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Karlsruhe Institute of Technology KIT, AstraZeneca
Authors: Haas-Santo, K. (Ekstern), Vankayala, B. (Ekstern), Dittmeyer, R. (Ekstern), Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Rozada-Sanchez, R. (Ekstern), Muller, F. (Ekstern)
Publication date: 2011
Event: Abstract from 8th European Congress of Chemical Engineering, Berlin, Germany.
Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

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 optimisation 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 data-sets 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.

General information
Distributed Parameter Modelling Applications

Here the issue of distributed parameter models is addressed. Spatial variations as well as time are considered important. Several applications for both steady state and dynamic applications are given. These relate to the processing of oil shale, the granulation of industrial fertilizers and the development of a short-path evaporator. The oil shale processing problem illustrates the interplay amongst particle flows in rotating drums, heat and mass transfer between solid and gas phases. The industrial application considers the dynamics of an Alberta-Taciuk processor, commonly used in shale oil and oil sands processing. The fertilizer granulation model considers the dynamics of MAP-DAP (mono and diammonium phosphates) production within an industrial granulator, that involves complex crystallisation, chemical reaction and particle growth, captured through population balances. A final example considers the steady state, distributed behaviour of a short-path evaporator.

General information

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Hukkerikar, A. (Intern), Sarup, B. (Ekstern), Abildskov, J. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2011
Event: Abstract from 2011 AIChE Annual Meeting, Minneapolis, MN, United States.
Main Research Area: Technical/natural sciences
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Crystallisation, Granulation, Spatial variation, Particle transport, Oil shale processing, Alberta-Taciuk Processor (ATP), Short-path evaporator, MAP-DAP, Daesim Dynamics, Population balances, Industrial fertilizers, Distributed parameter model

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Editors: Cameron, I., Gani, R.
Main Research Area: Technical/natural sciences

Editorial announcement

General information

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Authors: Gani, R. (ed.) (Intern)
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Efficient, Reliable and Predictive Solvent Design for Pharmaceutical Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, AstraZeneca
Authors: Conte, E. (Intern), Gani, R. (Intern), Crafts, P. A. (Ekstern), Sansonetti, S. (Intern)
Publication date: 2011
Event: Abstract from 2011 AIChE Annual Meeting, Minneapolis, MN, United States.
Main Research Area: Technical/natural sciences
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Estimation of Properties of Pure Components Using Improved Group Contribution Based and Atom Connectivity Index Based Models and Uncertainty Analysis

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
Authors: Hukkerikar, A. (Intern), Sarup, B. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2011
Main Research Area: Technical/natural sciences
Electronic versions:
prod21320327671411.AMH_ESAT_Abstract[1].pdf
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Source-ID: 312255
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Generic Model and Data Based Framework for Analysis and Development of Crystallization Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
Authors: Meisler, K. T. (Intern), Abdul Samad, N. A. F. (Intern), Gernaey, K. (Intern), von Solms, N. (Intern), Gani, R. (Intern)
Publication date: 2011
Event: Abstract from 2011 AIChE Annual Meeting, Minneapolis, MN, United States.
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Links:
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Heat-Integrated Reactive Distillation

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Argonne National Laboratory, ChemProcess Technologies, Tulane University
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.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abdul Samad, N. A. F. (Intern), Singh, R. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication: 2011

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Main Research Area: Technical/natural sciences
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**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.

**General information**

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Crystal size distribution, Multidimensional, Crystal shape
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**Interoperability between Modelling Tools (MoT) with Thermodynamic Property Prediction Packages (Simulis® Thermodynamics) and Process Simulators (ProSimPlus) Via CAPE-OPEN Standards**

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State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, ProSim S.A.
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern), Déchelotte, S. (Ekstern), Vacher, A. (Ekstern), Baudouin, O. (Ekstern)
Number of pages: 440
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Electronic versions:
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Lipid Processing Technology: Building a Multilevel Modeling Network

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; 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.

General information

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Technical University of Denmark, Alfa Laval Copenhagen A/S
Authors: Díaz Tovar, C. A. (Intern), Mustaffa, A. A. (Intern), Mukkerikar, A. (Ekstern), Quaglia, A. (Intern), Kontogeorgis, G. (Intern), Sarup, B. (Ekstern), Gani, R. (Intern)
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Process design, Property prediction models, Multilevel modeling, Computer aided flow sheet design, Lipid technology

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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 (eg. 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.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering, Alfa Laval Copenhagen A/S
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**Lipid Processing Technology: Shifting From Waste Streams to High-Value Commercial by-Products**

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering, Alfa Laval Copenhagen A/S
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**Lipid technology: Property prediction and process design/analysis in the edible oil and biodiesel industries**

In this work some of the property related issues in lipid processing technology employed in edible oil and biodiesel production are highlighted. This includes the identification of the most representative chemical species (acylglycerides, free fatty acids, tocopherols, sterols, carotenes, and fatty acid methyl esters); their representation and classification in terms of molecular structures; the collection of available experimental data of their pure component physical properties; the adoption of appropriate property-process models for the design and analysis of production processes through computer-aided tools like process simulation. Whenever experimental data were not available, the property models based on the group contribution approach (GC) was employed to fill-out the gaps in the database. This included pure component single-value properties (for example, the normal melting point temperature or the critical pressure) as well as temperature dependent properties (for example, vapor pressure, liquid density, and liquid viscosity). Whenever enough data was not available, the PC-SAFT EoS was used to generate pseudo-experimental data for the temperature dependent properties for regression of the GC-based model parameters. The filled database and property models have been employed through a process simulation to analyze the design issues of typical edible oil processes.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Alfa Laval Copenhagen A/S
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Methodology for Design and Analysis of Reactive Distillation Involving Multielement Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Jantharasuk, A. (Intern), Gani, R. (Intern), Assabumrungrat, S. (Ekstern), Górak, A. (Ekstern)
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Methodology for Design and Analysis of Reactive Distillation Involving Multielement Systems
A new methodology for design and analysis of reactive distillation has been developed. In this work, the element-based approach, coupled with a driving force diagram, has been extended and applied to the design of a reactive distillation column involving multielement (multicomponent) systems. The transformation of ordinary systems to element-based ones and the aggregation of non-key elements allow the important design parameters, such as the number of stages, feed stage and minimum reflux ratio, to be determined by using simple diagrams similar to those regularly employed for non-reactive systems consisting of two components. Based on this methodology, an optimal design configuration is identified using the equivalent binary-element-driving force diagram. Two case studies of methyl acetate (MeOAc) synthesis and methyl-tert-butyl ether (MTBE) synthesis have been considered to demonstrate the successful applications of the methodology. Moreover, energy requirements for various column configurations corresponding to different feed locatio

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Technische Universität Dortmund, Chulalongkorn University
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Web of Science (2016): Indexed yes
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Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
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Model-based engineering for product-process design - dealing with uncertainties

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sin, G. (Intern), Gani, R. (Intern)
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Main Research Area: Technical/natural sciences
Model based process-product design and analysis
This paper gives a perspective on modelling and the important role it has within product-process design and analysis. Different modelling issues related to development and application of systematic model-based solution approaches for product-process design is discussed and the need for a hybrid model-based framework is highlighted. This framework should be able to manage knowledge-data, models, and associated methods and tools integrated with design work-flows and data-flows for specific product-process design problems. In particular, the framework needs to manage models of different types, forms and complexity, together with their associated parameters. An example of a model-based system for design of chemicals based formulated products is also given.

Modeling and design of reacting systems with phase transfer catalysis
Issues related to the design of biphasic (liquid) catalytic reaction operations are discussed. A chemical system involving the reaction of an organic-phase soluble reactant (A) with an aqueous-phase soluble reactant (B) in the presence of phase transfer catalyst (PTC) is modeled and based on it, some of the design issues related to improved reaction operation are analyzed. Since the solubility of the different forms of the PTC in the organic solvent affects ultimately the catalyst partition coefficients, therefore, the organic solvent plays an important role in the design of PTC-based reacting systems. A model-based strategy for the selection of the best organic solvent/catalyst that improves the reaction operation is highlighted for the reacting system: benzyl chloride (A) and sodium bromide (B) reacting through tetrabutylammonium bromide (PTC).
Modeling and design of reacting systems with phase transfer catalysis

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State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Jealott's Hill International Research Center
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Publication date: 2011
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Thermodynamic modeling, Phase transfer catalysis, Process optimization, Reactor design
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Modelling and design of phase transfer catalytic processes

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Jealott's Hill International Research Center
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Main Research Area: Technical/natural sciences
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Modelling for Bio-, Agro- and Pharma-Applications

This chapter considers a range of modelling applications drawn from biological, agrochemical and pharma fields. Microcapsule controlled release of an active ingredient is considered through a time dependent model. Burst-time and lag-time effects are considered and the model adopts a multiscale approach for meso and microscale partial models. The specific case study of codeine release is examined. As a bio-application, a batch fermentation process is modelled. This involves the generation of a pre-cursor compound for insulin production. The plant involves a number of coupled unit operations such as mixers, fermenter as well as air compression and filtration. Milk pasteurisation is another application considered in this chapter. The intention is to look at the temperature profile of milk through the process, which has 4 distinct phases. Other case studies in this chapter include a dynamic model of a milling process within pharmaceutical production as well as a dynamic model representing a fluidised granulation bed for pharma products. The final model considers the tablet pressing process.

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Editors: Cameron, I., Gani, R.
Modelling: Nature and Use

Engineering of products and processes is increasingly “model-centric”. Models in their multitudinous forms are ubiquitous, being heavily used for a range of decision making activities across all life cycle phases. This chapter gives an overview of what is a model, the principal activities in the formation of a model for a specific purpose and the wide range of problem types that characterise the application areas of those models. In particular, a strong systems and life cycle perspective is presented which emphasises the development and application of models within each of the life cycle phases. The modelling goal is emphasised and discussed in terms of a triplet of: the model, a model application and the type of system under study. The much wider length and time scale phenomena now being addressed through modelling is discussed. This change has broadened modelling practice from a dominance on the mesoscale phenomena towards higher and lower scales. This breadth in scale-spread of the partial models being developed presents significant challenges around multiscale modelling and the integration frameworks for such complex system modelling. A number of these frameworks are given in the chapter and are discussed. Throughout the chapter a number of taxonomies around model types and forms help summarise the current modelling situation within much of product and process applications.

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Authors: Cameron, I. (Ekstern), Gani, R. (Intern)
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Modelling of Batch Process Operations
Here a batch cooling crystalliser is modelled and simulated as is a batch distillation system. In the batch crystalliser four operational modes of the crystalliser are considered, namely: initial cooling, nucleation, crystal growth and product removal. A model generation procedure is shown that sets out a clear set of steps to produce the model for dynamic simulation purposes. A population balance approach is adopted which through the application of a method of moments produces a set of ODEs from the original PDE model. A full analysis of the model is performed to generate the Degrees of Freedom (DoF) analysis, choice of variables to satisfy DoF and solution strategy. The batch distillation model for setting up and testing an operating sequence is developed and simulated. This looks at such operating policies as constant reflux ratio or set concentration of specific compound in the residue etc. A wide range of dynamic runs illustrates the effects of adopting certain operational policies.

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Modelling Practice
This chapter deals with the practicalities of building, testing, deploying and maintaining models. It gives specific advice for each phase of the modelling cycle. To do this, a modelling framework is introduced which covers: problem and model definition; model conceptualization; model data requirements; model construction; model solution; model verification; model validation and finally model deployment and maintenance. Within the adopted methodology, each step is discussed through the consideration of key issues and questions relevant to the modelling activity. Practical advice, based on many years of experience is providing in directing the reader in their activities. Traps and pitfalls are discussed and strategies also given to improve model development towards “fit-for-purpose” models. The emphasis in this chapter is the adoption and exercise of a modelling methodology that has proven very successful in many model building activities. It is vital that good methodologies are adopted for both thoroughness and efficiency purposes. Asking good questions for each modelling stage can aid in getting to effective and efficient solutions in modelling practice. Modelling is very much a ‘goal oriented’ activity, under constraints of system insight, time, cost and human resources. The George Box dictum that “all models are wrong, some are useful” should be coupled with the parsimony principle to ensure optimal outcomes.

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Models for Dynamic Applications
This chapter covers aspects of the dynamic modelling and simulation of several complex operations that include a controlled blending tank, a direct methanol fuel cell that incorporates a multiscale model, a fluidised bed reactor, a standard chemical reactor and finally a polymerisation reactor. These models help illustrate aspects of model formulation, the generation of the underlying assumptions about the systems, the degrees of freedom analysis and finally the solution and simulation of the models subject to changes in a variety of inputs. It is shown how an integrated system such as ICAS-MoT can be applied to formulate, analyse and solve these dynamic problems and how in the case of the fuel cell problem the model consists of coupled meso and micro scale models. It is shown how data flows are handled between the models and how the solution is obtained within the modelling environment.

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Publication date: 2011
Moving from batch towards continuous organic-chemical pharmaceutical production

Pharmaceutical ingredients have traditionally been produced in batches using multipurpose stirred vessels. Reactions and separations have typically been tailored to fit these units, facing multiple limitations when transferring synthetic routes from the laboratory to industrial scale. Scaling up thus resulted in many cases in low reaction yields and separation efficiencies. These limitations were however compensated by a relatively fast process implementation. For the pharmaceutical industry this meant that new drug products could be exclusively marketed for a longer time period, resulting in higher benefits than those that could be obtained with a highly optimized process requiring extra development time. Being the first to commercialize a product also meant a fundamental marketing advantage, since healthcare professionals commonly related pharmaceutical products to the original trademark. Furthermore, once a pharmaceutical product was approved, changes to the original production process could only be achieved at the expense of revalidating the whole process in a worldwide market, which typically prevented pharmaceutical companies from optimizing already existing manufacturing processes.

Today, however, the pharmaceutical industry is facing a globalized market where national health institutions increasingly favor the prescription of low-cost generics, and it is more and more expensive to develop new pharmaceutical ingredients with the potential to become, for a few years, blockbusters. Fierce competition has therefore resulted in a need to reduce manufacturing costs and optimize the efficiency of production processes. In addition, ethical reasons and ever stricter legislations demand the development of sustainable processes with the lowest possible environmental footprint. Continuous pharmaceutical manufacturing has been proposed as a way to facilitate process development and scale up, resulting in higher yields, improved quality, lower risks and reduced environmental impacts. Regulatory agencies, such as the FDA, have encouraged the transition towards novel technologies through increased process understanding. Developing a process within a more flexible design space based on sound engineering judgment potentially allows process optimization once the product has already been approved. Micro- and mini-chemical systems have been envisaged as the optimal scale for pharmaceutical production, due to improved heat and mass transfer allowing safer operation in a larger design space. Scaling up to high throughputs could then be performed by replicating small-scale units as required.

However, significant uncertainties arise. For example, when should continuous processes be selected? Where are the highest benefits found? How can a continuous process be designed and implemented? Are continuous processes compatible with slow reactions? Do they allow problem free processing of solid particles? What is the cost needed to implement a continuous process? This PhD thesis tries to answer some of those questions through the development of a systematic framework that takes advantage of continuous processing technologies and process systems engineering for the efficient design of continuous pharmaceutical processes. The framework consists of a step-by-step procedure that guides the user from drug discovery and the initial process development steps towards process implementation. Guidelines are suggested for the selection of the most suitable operating mode. Conceptual continuous processes can then be compared against traditional batch-wise processes in order to evaluate potential cost savings and/or lower environmental footprints.

The design framework has been applied to a process originally developed by H. Lundbeck A/S to produce zuclopenthixol, an active pharmaceutical ingredient. The synthetic process includes four reaction steps (alkylation by a Grignard reaction, hydrolysis of the alkoxide product, dehydration and hydroamination) with very different kinetics and thermodynamics, and several separation and solvent exchange steps. The implementation of continuous processes provided improved product quality without the need of some of the product isolation and purification steps, resulting in a significant simplification of the process. The process mass intensity (kg of raw materials used per kg of product obtained) could then be reduced to at least half the original value.

In this thesis, three of the unit operations included in the zuclopenthixol process were studied in detail. Specifically, the continuous alkylation reaction was achieved using a filter reactor coupled with a side-entry tubular reactor, using real-time in-line near-infrared (NIR) spectroscopy for monitoring the reaction and ensuring the right product quality. A subsequent hydrolysis of the alkoxide product was performed in continuous mode in a tubular reactor with segmented flow. The product of the hydrolysis reaction was fed to a hydrophobic membrane separator where the organic and aqueous phases were split. The organic phase was then dehydrated in continuous mode in a pressurized tubular reactor where the reaction rate of an otherwise slow reaction could be optimized by increasing the temperature above the normal boiling point of the solvent. These three unit operations could potentially be employed in similar reaction and separation steps, thus constituting ‘continuous-flow building blocks’ for the design of novel continuous pharmaceutical processes.
Optimal design of a multi-product biorefinery system

In this paper we propose a biorefinery optimization model that can be used to find the optimal processing route for the production of ethanol, butanol, succinic acid and blends of these chemicals with fossil fuel based gasoline. The approach unites transshipment models with a superstructure, resulting in a Mixed Integer Non-Linear Program (MINLP). We consider a specific problem based on a network of 72 processing steps (including different pretreatment steps, hydrolysis, fermentation, different separations and fuel blending steps) that can be used to process two different types of feedstock. Numerical results are presented for four different optimization objectives (maximize yield, minimize costs, minimize waste and minimum fixed cost), while evaluating different cases (single product and multi-product).
Optimal Design of Ionic Liquid Entrainers for Extractive Distillation of Azeotrope Systems

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, University of Kansas
Authors: Roughton, B. C. (Ekstern), White, J. (Ekstern), Gani, R. (Intern), Camarda, K. V. (Ekstern)
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Overview of the Case Studies
A series of case studies are used to illustrate many of the underlying modelling principles within the book. To facilitate this, the ICAS-MoT modelling tool has been used. A wide range of application areas have been chosen to ensure that the principal concepts of effective and efficient modelling are exercised. Conceptual frameworks for single and multiscale problems are given and explained. The importance of the steps is also explained, through annotated schematic diagrams. The important issues around workflow and data flow are given in diagrammatic form.

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Parameter Estimation
In this chapter the importance of parameter estimation in model development is illustrated through various applications related to reaction systems. In particular, rate constants in a reaction system are obtained through parameter estimation methods. These approaches often require the application of optimisation techniques coupled with dynamic solution of the underlying model. Linear and nonlinear approaches to parameter estimation are investigated. There is also the application of maximum likelihood principles in the estimation of parameters, as well as the use of orthogonal collocation to generate a set of algebraic equations as the basis for parameter estimation. These approaches are illustrated using estimations of kinetic constants from reaction system models.

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Phenomena-based Process Synthesis and Design to achieve Process Intensification

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State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Phenomena-based Process Synthesis and Design to achieve Process Intensification

In order to improve processes incorporating process intensification and to allow them to go beyond pre-defined unit operations, the process has to be viewed at a lower level of aggregation, namely the phenomena scale. In this contribution, an approach for aggregating processes through phenomena building blocks in a systematic methodology is presented. First, all potential phenomena are identified, and then synthesized to phenomena-based flowsheets which are then screened against pre-defined constraints before the most promising options are identified, optimized and verified at the unit operation level. This phenomena-based synthesis/design methodology is tested through a case study.

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Phenomena-Based Process Synthesis and Design to Achieve Process Intensification

In recent years, Process Intensification (PI) has attracted considerable interest as a potential means of process improvements and to meet the increasing demands for sustainable production. PI aims to improve processes by increasing efficiency, reducing energy consumption, operational costs, volume, and waste as well as simplifying the flowsheet. A variety of intensified operations and equipment has been developed. Potentially, this creates a large number of options for possible process improvement, however, to date only a limited number of intensified technologies have achieved implementation, such as reactive distillation, dividing wall columns and reverse flow reactors [1]. One major reason for this is that the identification of the best PI option is neither simple nor systematic. In previous work [2] we reported the development of a general computer-aided systematic synthesis and design methodology in which redundant intensified options are systematically removed by checking against predefined constraints through a decomposition approach of a superstructure optimization problem. In this approach lower level steps employ simple and easy calculations, while the higher level steps employ more rigorous and detailed calculations. However, up to now, this methodology is limited to already reported PI unit operations which can be retrieved, together with all information necessary for synthesis and design of each of them, from a knowledge base tool. In order to invent new unit operations going beyond those currently in existence, process synthesis and design incorporating PI needs to be investigated at the phenomenological level [3, 4] which will be presented in this contribution. The basis of the phenomena-based process synthesis is transfer units consisting of mass, component, energy and momentum balances as well as phenomena building blocks and model equations describing them. Following the same rationale as the general methodology described previously, the problem is first defined, given a set of product quality and quantity as well as additional process constraints in addition to the potential need for the improvement. Next, the given information is analyzed to identify all potential phenomena building blocks. In the next step, the phenomena building blocks are joined together according to combination rules to match process intensification targets defined through a superstructure of flowsheet options. Based on these, the generated options are screened through performance specifications before unit operations are identified. For example, a counter-current sequence of similar simultaneous mixing and vapour-liquid phenomena with the final steps at both ends being simultaneous heat transfer, mixing and vapour-liquid phase change phenomena can be identified as a distillation
In the penultimate step, the remaining options are optimized with respect to a defined objective function. The results are verified through rigorous model simulations in the final step. The advantage of the phenomena-based process synthesis and design is that it generates potentially novel process options because the initial search space is wider than the search space of existing units (truly predictive models lead to reliable predictive solutions) as well as the simultaneous development of the necessary process models. In this contribution the application of a phenomena-based process synthesis combined with a systematic methodology through a computer-aided framework will be described and highlighted with selected examples in the area of distillation systems, together with a focus on some of the suitable methods and tools.

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Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
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Product and Process Modelling: A Case Study Approach
This book covers the area of product and process modelling via a case study approach. It addresses a wide range of modelling applications with emphasis on modelling methodology and the subsequent in-depth analysis of mathematical models to gain insight via structural aspects of the models. These approaches are put into the context of life cycle modelling, where multiscale and multiform modelling is increasingly prevalent in the 21st century. The book commences with a discussion of modern product and process modelling theory and practice followed by a series of case studies drawn from a variety of process industries. The book builds on the extensive modelling experience of the authors, who have developed models for both research and industrial purposes. It complements existing books by the authors in the modelling area. Those areas include the traditional petroleum and petrochemical industries to biotechnology applications, food, polymer and human health application areas. The book highlights to important nature of modern product and process modelling in the decision making processes across the life cycle. As such it provides an important resource for students, researchers and industrial practitioners.

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Property Modelling for Applications in Chemical Product and Process Design
Physical-chemical properties of pure chemicals and their mixtures play an important role in the design of chemicals based products and the processes that manufacture them. Although, the use of experimental data in design and analysis of chemicals based products and their processes is desirable, they are not always available. Also, it may be too expensive to measure them or it may take too much time. In these situations and when repetitive calculations are involved (as in process simulation), it is useful to have appropriate models to reliably predict the needed properties. A collection of methods tools such as database, property model library, model parameter regression, and, property-model based product-process design will be presented. The database contains pure component and mixture data for a wide range of organic chemicals. The property models are based on the combined group contribution and atom connectivity approach, called the GC-plus approach. This approach has been used to predict single value pure component properties, mixture properties of organic chemicals as well as average properties of polymer repeat units. An important feature of the GC-plus approach is that when a group parameter is missing, the atom connectivity based model is employed to predict the missing group interaction. In this way, a wide application range of the property modeling tool is ensured. Based on the property models,
targeted computer-aided techniques have been developed for design and analysis of organic chemicals, polymers, mixtures as well as separation processes. The presentation will highlight the framework (ICAS software) for property modeling, the property models and issues such as prediction accuracy, flexibility, maintenance and updating of the database. Also, application issues related to the use of property modeling tools in design and analysis of chemical product-process design, including biochemical processes will be highlighted.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
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Rational Design of Pharmaceutical and Other Liquid Formulations

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, AstraZeneca
Authors: Conte, E. (Intern), Sansonetti, S. (Intern), Crafts, P. A. (Ekstern), Gani, R. (Intern)
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Robust Market Launch Planning for a Multi- Echelon Pharmaceutical Supply Chain
It is well known, that the pharmaceutical industry is struggling with increasing cost and length of R&D projects. Earnings of a drug drop drastically after patent expiration. Thus, the industry spends much effort on reducing Time-to-Market. In the literature, little attention is given to drug launching activities after the drug has been approved. In this paper, we present a recourse-based stochastic model, which allows for time phasing the market entries to balance the fluctuating demand with the fixed and periodic production of the active pharmaceutical ingredient. The two major risk elements during launch are forecasting inaccuracy and the risk of a required label change from local regulatory authorities. Robust solutions are found by implementing the Robust Optimization framework.

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Organisations: Operations Management, Department of Management Engineering, Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Technische Universität München
Authors: Hansen, K. R. N. (Intern), Grunow, M. (Ekstern), Gani, R. (Intern)
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Selection of Prediction Methods for Thermophysical Properties for Process Modeling and Product Design of Biodiesel Manufacturing

To optimize biodiesel manufacturing, many reported studies have built simulation models to quantify the relationship between operating conditions and process performance. For mass and energy balance simulations, it is essential to know the four fundamental thermophysical properties of the feed oil: liquid density (ρL), vapor pressure (Pvap), liquid heat capacity (CPL), and heat of vaporization (ΔHvap). Additionally, to characterize the fuel qualities, it is critical to develop quantitative correlations to predict three biodiesel properties, namely, viscosity, cetane number, and flash point. Also, to ensure the operability of biodiesel in cold weather, one needs to quantitatively predict three low-temperature flow properties: cloud point (CP), pour point (PP), and cold filter plugging point (CFPP). This article presents the results from a comprehensive evaluation of the methods for predicting these four essential feed oil properties and six key biodiesel fuel properties. We compare the predictions to reported experimental data and recommend the appropriate prediction methods for each property based on accuracy, consistency, and generality. Of particular significance are (1) our presentation of simple and accurate methods for predicting the six key fuel properties based on the number of carbon atoms and the number of double bonds or the composition of total unsaturated fatty acid methyl esters (FAMEs) and (2) our posting of the Excel spreadsheets for implementing all of the evaluated accurate prediction methods on our group Web site (www.design.che.vt.edu) for the reader to download without charge.

General information
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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Virginia Polytechnic Institute and State University
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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Simultaneous Design of Ionic Liquids and Azeotropic Separation for Systems Containing Water

Separation of azeotropic mixtures is a very common but challenging task, covering a wide range of industrial sectors and issues. For example, most down-stream separation problems following a synthesis step of pharmaceutical and/or biochemical processes, involve the separation of azeotropes. Also, many separation tasks in the petrochemical and chemical industries involve separation of azeotropic mixtures. A common issue with the design and operation of these separation tasks is whether or not to use solvents? And, if solvents are to be used, what kind of solvent should be used and what would environmental impact would they cause? Ionic liquids show great promise for solvent-based separation, particularly for extractive distillation-based separations, due to their negligible vapor pressures and the fact that a wide range of solubilities and other properties can be obtained through structural changes. Since a large number of azeotropes encountered include water as one of the compounds, the use of ionic liquids in solvent-based separation of water in azeotropic systems has been investigated. Along with the design of the ionic liquid being used to entrain water, the extractive distillation process has also designed as an integrated ionic liquid–extractive process design. Based on the separation desired (for example, remove the water), an ionic liquid solvent and the separation process is designed or selected from a library of designed solutions, based upon the methodology that has been developed. In order to design ionic liquids with specific physical property values, a class of predictive property estimation models is required. In this work, a group contribution approach has been developed to predict the solvent-related properties of ionic liquids, highlighted by the Hildebrand solubility parameter and a special UNIFAC group contribution method for ionic liquids. The Hildebrand solubility parameter group contribution model was compared to reported literature values for the solubility parameter of several ionic liquids. The model showed good agreement with a maximum deviation of 15% and a root mean square difference of 1.56 MPa½. The predicted solubility parameters were then used to screen for ionic liquids that are soluble with water. The predicted solubility parameters ranged in value from 19.1 to 29.8 MPa½. Experimental solubility
data has been compared to the parameter values to check for consistency. The ionic liquid UNIFAC model was developed for a selected set of ionic liquid cations and anions. Group volume and area parameters were calculated using a three step procedure. First, the rules of Bondi were used for any applicable molecular groups within the cation or anion. Next, existing UNIFAC main group parameters were used for remaining undefined groups. Finally, reported literature values for the group volume and area parameters were used for any groups that still had not been defined. From experimental values for the activity coefficient at infinite dilution, group interaction parameters were fitted for the newly defined ionic liquid groups. The ionic liquid UNIFAC model was used to predict vapor-liquid equilibria for several aqueous azeotropic systems. The ionic liquids were evaluated for use as an entrainer for water in binary azeotropic mixtures where the mole fraction of water at the azeotrope is less than 30%. For promising ionic liquid candidates, the extractive distillation processes were designed using a reverse simulation approach and characterized in terms of the driving force (calculated from the predicted vapor-liquid equilibria) that corresponds to the optimal design of the separation process (in terms of number of stages, feed plate location, energy used, solvent loss, environmental impact, etc.). To ensure the feasibility of ionic liquids to be used as industrial entrainers, a correlation was also made relating molecular structure to thermal decomposition temperature. For any new synthesis-design problem involving aqueous azeotropes, all it now requires is to find the azeotropic composition of water and based on it, to identify an appropriate ionic liquid. Then the driving force is calculated for the azeotropic ionic liquid and based on it, the design of the extractive distillation process is retrieved from the database. The presentation will highlight the methodology, the tools and solutions from several case studies.

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Simultaneous Design of Ionic Liquids and Azeotropic Separation Processes
A methodology for the design of azeotrope separation processes using ionic liquids as entrainers is outlined. A Hildebrand solubility parameter group contribution model has been developed to screen for or design an ionic liquid entrainer that is soluble with the azeotropic components. Using the best candidate, vapor-liquid equilibria data is predicted using a new ionic liquid UNIFAC model that has been developed. The UNIFAC model is used to confirm the breaking of the azeotrope. The methanol-acetone azeotrope at 1 atm is used as an example. The azeotrope was predicted to break with 10 mol % [BMPy][BF4] added. The driving force concept is used to design an extractive distillation process that minimizes energy inputs. The methodology given can be expanded to the use of ionic liquids as entrainers in any azeotropic system of interest.

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Steady-State Process Modelling
This chapter covers the basic principles of steady state modelling and simulation using a number of case studies. Two principal approaches are illustrated that develop the unit operation models from first principles as well as through application of standard flowsheet simulators. The approaches illustrate the "equation oriented" approach as well as the "sequential modular" approach to solving complex flowsheets for steady state applications. The applications include the Williams-Otto plant, the hydrodealkylation (HDA) of toluene, conversion of ethylene to ethanol and a bio-ethanol process.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, University of Queensland
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Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Computer Aided Process Engineering Center
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Substrates adoption methodology (SAM) to achieve "Fast, Flexible, Future (F3)" pharmaceutical production processes
There is a significant cost associated with process development of a portfolio of pharmaceutical products, few of which will reach the market. Continuous processing will increase the "chemical space" which can increase development efficiency. For example one, particularly attractive option is to develop manufacturing processes based on modular continuous systems; a flexible generic continuous modular plant which can be adapted for different substrates. In the work reported here, a substrates adoption methodology (SAM) has been developed. The proposed SAM identifies the necessary changes to a template recipe & flowsheet in order to adapt it for a given substrate. The changes can be related to reagents (e.g. reducing agent, solvent, catalyst), process conditions (e.g. operating temperature, flow rates), as well as in the physical arrangement (configuration) of the modular process equipment within the template. In this way the substrates adoption methodology helps to achieve "fast, flexible, future (F3)" pharmaceutical production processes by adapting a recently designed generic modular process-plant. The supporting tools for the substrate adoption are: (1) an ontological knowledge-base consisting of the properties of substances, reaction characteristics and characteristics of unit operations; and (2) a model library consisting of the mathematical models. The objective of this presentation is two-fold: First to highlight the substrates adoption framework and the associated models, methods and tools, and second to demonstrate its applications using a pharmaceutical manufacturing case study involving the nitro reduction of 2-Nitro-4' - chlorodiphenylamine.
Systematic computation of phase partition and solubilities in phase transfer catalytic processes

Phase transfer catalysis (PTC) is a general methodology applicable to a great variety of reactions in which inorganic anions react with organic compounds. In PTC, reactions are performed in heterogeneous two phase systems in which there is a negligible mutual solubility of the phases. One aqueous phase serves as a reservoir of reacting anions, whereas organic reactants are located in a second, organic phase. The key feature of this approach is the use of a catalytic amount of an organic soluble cation (often a quaternary ammonium cation) to induce solubilization of the reactive anion in the organic phase while trying to minimize the partition of the product anion. Therefore the determination of the solubility and the related equilibrium partitioning of the active and inactive form of the PT catalyst between the two phases is critical for the design of successful phase transfer catalytic processes.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Jealott's Hill International Research Center
Systematic Engineering Approach to Development and Identification of Physiologically-Based Pharmacokinetic Models

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, University of Illinois at Chicago
Authors: Hall, C. (Ekstern), Sin, G. (Intern), Gani, R. (Intern), Linninger, A. (Ekstern)
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**Systematic methods for synthesis and design of sustainable chemical and biochemical processes**

Chemical and biochemical process design consists of designing the process that can sustainably manufacture an identified chemical product through a chemical or biochemical route. The chemical product tree is potentially very large; starting from a set of basic raw materials (such as petroleum, biomass, coal, natural gas, rock, etc., that are usually extracted), to a bigger set of basic chemical products (such as, ethylene, benzene, sulfuric acid, ammonia, etc., that are produced in large quantities), to an even bigger set of intermediates (such as, methanol, urea, succinic acid, ethylene glycol, etc., that are produced from the basic chemicals), to a very large number of refined chemicals and consumer products (where the chemical selected as the active ingredient is usually used in small quantity). At the top, the chemical products are usually from the life sciences, pharmaceutical, food and related industries and their development is principally based on experiment-based trial and error approaches. At the lower-middle end, the chemical products usually from the oil, petrochemical and chemical industries and use of model based tools in their development is quite common.

Using raw materials from the renewable resources, the sustainability of the product and therefore the process can be improved. Also, the number of alternatives that exist provide opportunities and challenges to find the best synthesis routes, for example, for process intensification or a multi-product processing complex like a biorefinery. The process synthesis design problem can be formulated as one where first a synthesis-design target (a process with desired qualities) is defined and then design alternatives (process flowsheets for different raw material-product connection) that match the target are identified and ordered according to a performance index. One way to achieve this, is to derive a generic mathematical formulation of the synthesis-design problem and then to decompose it into a set of easily manageable and solvable sub-problems. The sub-problems are solved according to a hierarchy that gradually decreases the number of feasible alternatives. The final step involves solving a well-defined optimization problem or simply ordering the feasible solutions according to defined performance criteria to determine the optimal solution. This synthesis-design approach is suitable for problems that are highly non-linear, contain models and data from different sources, has a large combinatorial problem size, and/or require the use of multiple methods and tools. The decomposition based “define target – match target” approach to process synthesis-design has been converted into model-based computer-aided tools for process intensification, sustainable process design, identification of optimal biorefinery models as well as integrated process-control design, and chemical product design. The lecture will present the main concepts, the decomposition based solution approach, the developed methods and tools together with illustrative examples covering chemical and biochemical process synthesis and design.

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
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Systematic Modelling and Crystal Size Distribution Control for Batch Crystallization Processes

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.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abdul Samad, N. A. F. (Intern), Singh, R. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
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Systematic multi-scale model development strategy for fragrance spraying process and transport

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Firmenich Inc.
Authors: Heitzig, M. (Intern), Gregson, C. (Ekstern), Sin, G. (Intern), Gani, R. (Intern)
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.

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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.

**Tailor-made Design of Chemical Blends using Decomposition-based Computer-aided Approach**

Computer aided technique is an efficient approach to solve chemical product design problems such as design of blended liquid products (chemical blending). In chemical blending, one tries to find the best candidate, which satisfies the product targets defined in terms of desired product attributes (properties). In this way, first the systematic computer-aided technique establishes the search space, and then narrows it down in subsequent steps until a small number of feasible and promising candidates remain and then experimental work may be conducted to verify if any or all the candidates satisfy the desired product attributes. Alternatively, rigorous modelling could also be used in this final step. In other words, the candidates are quickly generated and screened until a small number is left for final selection and evaluation by experiment and/or rigorous modelling. This paper presents a design methodology for blended liquid products that identifies a set of feasible chemical blends. The blend design problem is formulated as a nonlinear programming (NLP) model where the objective is to find the optimal blended gasoline or diesel product subject to blend chemicals and their compositions, a set of desired properties of the product as design constraints. The blend design problem is solved using a decomposition approach, which eliminates infeasible and/or redundant candidates gradually. The decomposition method reduces the search space in a systematic way. This general blend design problem is decomposed into two stages. The first stage investigates the mixture stability where all unstable mixtures are eliminated and the stable blend candidates are retained for further testing. In the second stage, the blend candidates have to satisfy a set of target properties that are ranked according to a specified priority. Finally, a short list of candidates, ordered in terms of specified performance criteria, is produced for final testing and selection. This systematic and computer-aided approach is illustrated through a case study involving the design of blends of gasoline with oxygenates from biomass for use in internal combustion engines. The blend design formulation is able to find the optimal blend candidate.

**Tennessee Eastman Plant-wide Industrial Process Challenge Problem**

This chapter presents a comprehensive analysis and modelling of the Tennessee Eastman challenge problem. Both a simplified model of the system as well as a full process model that includes the energy balances is given. In each case a full model analysis is carried out to establish the degrees of freedom (DoF) and the appropriate selection of variables to satisfy the DoF. Of major concern is the control of the process. The chapter considers the open-loop dynamics of the flowsheet as well as the closed loop responses. Plots show the reactor dynamic behaviour as well as stripper exit flowrates. All problem data are given and initial conditions for dynamic runs are stated to enable readers to replicate the model performance.
The Chameleonic Behavior of Ionic Liquids and its Impact on the Solubility Parameters Estimation

The possibility to develop a solubility parameter scale, with the purpose of predicting the performance and help the selection of ILs, is here evaluated. For the estimation of solubility parameters, infinite dilution activity coefficient data is used. The results allowed the identification of a curious behavior for the ILs that seem to present more than one solubility parameter acting as polar molecules in some situations and as non-polar molecules in others, depending on the medium. This behavior was confirmed by solubility measurements of [C4MIM][PF6] in solvent mixtures. The solubility parameters were alternatively estimated based on other properties, namely viscosities and enthalpies of vaporization, and the relation between the various sets of solubility parameters is discussed. The results obtained suggest that, given the complexity of IL molecules and their liquid phase, a one-dimensional solubility parameter scale able to characterize these fluids is not feasible.

General information
State: Published
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The virtual product-process design laboratory to manage the complexity in the verification of formulated products

Formulations are complex products since active ingredients, solvents and additives are combined together to obtain a product with several functions and properties. When designing/verifying a formulated product, the required modelling effort is challenging as properties and functions of complex mixtures need to be predicted. This complexity has to be managed through decomposition of the problem into sub-problems. Each sub-problem is solved and analyzed and, from the knowledge gained, an overall evaluation of the complex chemical system representing the product is made. The virtual Product-Process Design laboratory (virtual PPD-lab) software is based on this decomposition strategy for the design of formulated liquid products. When the needed models are available in the software, the solution of formulation design/verification problems is straightforward, while when models are not available in the software library, they need to be developed and/or implemented. The potential of the virtual PPD-lab in managing the complexity in the verification of formulated products, after the needed models have been developed and implemented, is highlighted in this paper through a case study from industry dealing with the verification of a hair spray product.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Akzo Nobel Functional Chemicals AB
Innovation in Integrated Chemical Product-Process Design - Development through a Model-based Systems Approach

The ‘consumer oriented chemicals based products’ such as shampoos, sunscreens, insect repellents are used everyday by millions of people. They are structured products, constituted of numerous chemicals. This complexity gives the reason for which mainly experimental techniques are still employed in the design and verification of such products. The objective of this project is to tackle the problem with computer-aided tools at first, using experimental techniques for final testing, evaluation and amendment. In this way, time and resources can be spared and the product can reach the market faster and at a reduced cost. The main contribution of this project is the development of an integrated methodology for the design and verification of formulated products. The methodology includes a first stage in which computer-aided techniques are employed to determine the base case product formula, a second stage in which experiments are planned and a third stage in which experiments are performed to validate the final product formula. The main focus of the project is on the development of the computer-aided stage of the methodology described above. The methodology considers two different scenarios: the design of new products and the verification of modified and/or existing products. In the design scenario, since the identity of the chemicals belonging to the formulated product is unknown, and, thousands of design alternatives may be generated, the problem may encounter a combinatorial explosion unless appropriate model-based screening techniques are employed. In the verification scenario, a shortlist of candidate ingredients is provided, therefore the problem size is much smaller and rigorous property models can be employed/developed. When using computer-aided tools for product design, several issues need to be addressed: new property models may need to be developed and/or the application range of existing property models may need to be extended (that is, new model parameters are needed), new and more efficient methods and tools for the application of the models may need to be developed, together with a flexible framework, which collects the methods and tools and allows their use in an integrated way. All these issues are addressed in this PhD project: new property models for the estimation of the target properties are developed; two algorithms for the design of binary mixtures and for the stability test of liquid systems are proposed, and the associated computer programs are also developed; the computer-aided stage of the methodology for formulation design and verification is implemented as an option in the software the ‘virtual Product-Process Design laboratory’. Four case studies have been developed to illustrate the use of the proposed methodology. For two of these case studies the complete methodology has been applied, that is, including the stages of experimental planning and experimental testing/amendment. For the other two, only the computer-aided stage has been applied.
Are safe results obtained when the PC-SAFT equation of state is applied to ordinary pure chemicals?

The PC-SAFT equation of state is a very popular and promising model for fluids that employs a complicated pressure-explicit mathematical function (and can therefore not be solved analytically at a specified pressure and temperature, contrary to classical cubic equations). In this work, we demonstrate that in case of pure fluids, the PC-SAFT equation may exhibit up to five different volume-roots whereas cubic equations give at the most three volume-roots (and yet, only one or two volume roots have real significance). The consequence of this strongly atypical behaviour is the existence of two different fluid-fluid coexistence lines (the vapour pressure-curve and an additional liquid-liquid equilibrium curve) and two critical points for a same pure component, which is obviously physically inconsistent. In addition to n-alkanes, nearly sixty very common pure components (branched alkanes, cycloalkanes, aromatics, esters, gases, and so on) were tested out and without any exception, we can claim that all of them exhibit this undesired behaviour. In addition, such similar phenomena (i.e. existence of more than three volume-roots) may also arise with mixtures. From a computational point of view, most of the algorithms used for solving equations of state only search for three roots at the most and are thus likely to be inefficient when an equation of state gives more than three volume-roots. To overcome this limitation, a simple procedure allowing to identify all the possible volume-roots of an equation of state is proposed.
Process-product synthesis, design and analysis through the Group Contribution (GC) approach

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Alvarado-Morales, M. (Intern), Gani, R. (Intern)
Publication date: Jul 2010

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PEC10-13.pdf
Source: orbit
Source-ID: 255439
A computer-aided framework for regression and multi-scale-modelling needs in innovative product-process engineering

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

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265224
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

A computer-aided framework for regression and multi-scale-modelling needs in innovative product-process engineering

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Heitzig, M. (Intern), Sin, G. (Intern), Glarborg, P. (Intern), Gani, R. (Intern)
Pages: 379-384
Publication date: 2010

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Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 28
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Series: Computer - Aided Chemical Engineering
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 20th European Symposium on Computer Aided Process Engineering, Ischia, Italy, 06/06/2010 - 06/06/2010
Links: http://www.elsevierdirect.com/product.jsp?isbn=9780444535696&dmnum=CWS1
Source: orbit
Source-ID: 255445
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010


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

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265931
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

A computer-aided modelling framework for use in product-process engineering
A Generic Model-Based Framework for Batch Cooling Crystallization Processes

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.

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

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.
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<td>SNIP 1.113</td>
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A model-based systems approach to pharmaceutical product-process design and analysis

This is a perspective paper highlighting the need for systematic model-based design and analysis in pharmaceutical product-process development. A model-based framework is presented and the role, development and use of models of various types are discussed together with the structure of the models for the product and the process. The need for a systematic modelling framework is highlighted together with modelling issues related to model identification, adaptation and extension. In the area of product design and analysis, predictive models are needed with a wide application range. In the area of process synthesis and design, the use of generic process models from which specific process models can be generated, is highlighted. The use of a multi-scale modelling approach to extend the application range of the property models is highlighted as well. Examples of different types of process models, model analysis and model generation are presented.
Analysis and application of GC plus models for property prediction of organic chemical systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mustaffa, A. A. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265207
Publication: Research - peer-review › Poster – Annual report year: 2010

An Ontological Knowledge-Based System for Identification of Efficient Chemical Production Routes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 268891
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010
An ontological knowledge based system for selection of process monitoring and analysis tools

Efficient process monitoring and analysis tools provide the means for automated supervision and control of manufacturing plants and therefore play an important role in plant safety, process control and assurance of end product quality. The availability of a large number of different process monitoring and analysis tools for a wide range of operations has made their selection a difficult, time consuming and challenging task. Therefore, an efficient and systematic knowledge base coupled with an inference system is necessary to support the optimal selection of process monitoring and analysis tools, satisfying the process and user constraints. A knowledge base consisting of the process knowledge as well as knowledge on measurement methods and tools has been developed. An ontology has been designed for knowledge representation and management. The developed knowledge base has a dual feature. On the one hand, it facilitates the selection of proper monitoring and analysis tools for a given application or process. On the other hand, it permits the identification of potential applications for a given monitoring technique or tool. An efficient inference system based on forward as well as reverse search procedures has been developed to retrieve the data/information stored in the knowledge base.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Pages: 1137-1154
Publication date: 2010
Main Research Area: Technical/natural sciences

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Journal: Computers & Chemical Engineering
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Ratings:
  BFI (2017): BFI-level 2
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 2
  Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 2
  Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
  ISI indexed (2011): ISI indexed yes
  Web of Science (2011): Indexed yes
  BFI (2010): BFI-level 2
  Scopus rating (2010): SJR 1.176 SNIP 1.796
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 2
  Scopus rating (2009): SJR 1.154 SNIP 2.166
  Web of Science (2009): Indexed yes
  BFI (2008): BFI-level 2
  Scopus rating (2008): SJR 1.293 SNIP 2.127
Application of a Synthesis and Design Methodology Incorporating Process Intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Publication information
Original language: English
Source: orbit
Source-ID: 255447
Publication: Research - peer-review › Journal article – 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
Authors: Abd.Hamid, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 148-149
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Main Research Area: Technical/natural sciences
Conference: 3. Dansk KemiingeniørKonference, Kgs. Lyngby, Denmark, 16/06/2010 - 16/06/2010
Source: orbit
Source-ID: 266240
Publication: Research › Article in proceedings – Annual report year: 2010
Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problems for Reactor-Separator-Recycle System

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, \( A \rightarrow B \rightarrow C \) 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.

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

Host publication information
Title of host publication: Proceedings of 9th International Symposium on Dynamics and Control of Process Systems
Main Research Area: Technical/natural sciences
Conference: 9th International Symposium on Dynamics and Control of Process Systems, Leuvren, Belgium, 05/07/2010 - 05/07/2010
Source: orbit
Source-ID: 265043
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010


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

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265119
Publication: 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
Authors: Abd.Hamid, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Application of Solid Resins for Controlled Substrate supply to biocatalytic reactions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Al-Haque, N. (Intern), Tufvesson, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010
Event: Poster session presented at BEST 2010, Bologna, Italy.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 267263
Publication: Research - peer-review › Poster – Annual report year: 2010

A process systems engineering approach to managing the complexity in chemical product process design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265926
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

A systematic methodology to synthesize/design processes, incorporating process intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Jensen, J. S. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 267045
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

A systematic synthesis and design methodology to achieve process intensification for multi-phase reactions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Jensen, J. S. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010
Event: Poster session presented at 19th International Congress of Chemical and Process Engineering and 7th European Congress of Chemical Engineering, Prague, Czech Republic.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 267048
Publication: Research › peer-review › Poster – Annual report year: 2010
A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes

**General Information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Román-Martínez, A. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2010

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265223
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes

Process intensification (PI) has the potential to improve existing processes or create new process options which are needed in order to produce products using more sustainable methods. PI creates an enormous number of process options. In order to manage the complexity of options in which a feasible and optimal process solution may exist, the application of process synthesis tools results in the development of a systematic methodology to implement PI. Starting from an analysis of existing processes, this methodology generates a set of feasible process options and reduces their number through a number of screening steps until from the remaining feasible options, the optimal is found. The application of this systematic methodology through a computer-aided framework is presented through a case study, the chemo-enzymatic synthesis of N-acetyl-D-neuraminic acid (Neu5Ac).

**General Information**
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Román-Martínez, A. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Pages: 241-246
Publication date: 2010

**Host publication information**
Title of host publication: Proceedings of the 20th European Symposium on Computer Aided Process Engineering
Publisher: Elsevier Science
Series: Computer - Aided Chemical Engineering
Volume: 28
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 20th European Symposium on Computer Aided Process Engineering, Ischia, Italy, 06/06/2010 - 06/06/2010
Methodology, Process synthesis, Process intensification, Biocatalysis, N-acetyleneuraminic acid (Neu5Ac)
DOI:
10.1016/S1570-7946(10)28041-0
Source: orbit
Source-ID: 255431
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

**CAPEC Research Report 2010**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2010

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PEC10-25-capec-research-report.pdf
Source: orbit
Source-ID: 265052
Computer-aided design of ionic-liquids by group contribution methods

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Aguirre, C. (Ekstern), Cisternas, L. (Ekstern), Gani, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265206
Publication: Research - peer-review › Poster – Annual report year: 2010

Computer aided model based design and analysis of hybrid membrane reaction, separation process

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Soni, V. (Intern), Mitkowski, P. T. (Intern)
Number of pages: 1,570
Publication date: 2010
Host publication information
Title of host publication: Comprehensive Membrane Science and Engineering: Chemical and biochemical transformations in membrane systems
Volume: Book 3 Section 1 Part 3
Publisher: Elsevier Science
Editor: Drioli, E.
ISBN (Print): 978-0-444-53204-6
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 264505
Publication: Research - peer-review › Book chapter – Annual report year: 2010

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
Authors: Heitzig, M. (Intern), Sin, G. (Intern), Glarborg, P. (Intern), Gani, R. (Intern)
Pages: 171-172
Publication date: 2010
Host publication information
Title of host publication: Proceedings of Dansk Kemiingenierkonference 2010
Main Research Area: Technical/natural sciences
Conference: 3. Dansk KemiingenierKonference, Kgs. Lyngby, Denmark, 16/06/2010 - 16/06/2010
Source: orbit
Source-ID: 266241
Publication: Research › Article in proceedings – Annual report year: 2010

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
Authors: Heitzig, M. (Intern), Sin, G. (Intern), Glarborg, P. (Intern), Gani, R. (Intern)
Publication date: 2010
Computer aided molecular and blend design applied to fuel-related products (Invited Lecture)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266268
Publication: Research › Poster – Annual report year: 2010

Computer aided polymer design using multiscale modeling

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Abildskov, J. (Intern), Gani, R. (Intern), Tsolou, G. (Ekstern), Mavrantzas, V. G. (Ekstern)
Pages: 369-380
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Brazilian Journal of Chemical Engineering
Volume: 27
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Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.429 SNIP 0.965 CiteScore 1.46
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.426 SNIP 0.967 CiteScore 1.29
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.411 SNIP 0.851 CiteScore 1.3
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.449 SNIP 0.91 CiteScore 1.26
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.465 SNIP 0.864 CiteScore 1.04
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.401 SNIP 0.75 CiteScore 1.23
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.387 SNIP 0.708
Web of Science (2010): Indexed yes
Design and synthesis of sustainable chemical and biochemical processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 268439
Publication: Research › Article in proceedings – Annual report year: 2010

Design challenges and sustainability issues in gas processing: A view from academia (Invited Lecture)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265111
Publication: Research › Article in proceedings – Annual report year: 2010

Design of batch operations: Systematic methodology for generation and analysis of sustainable alternatives
The objective of this paper is to present a new methodology that is able to generate, screen and identify sustainable alternatives to continuous chemical processes as well as processes operating in the batch mode. The methodology generates the sustainable (design) alternatives by locating the operational, environmental, economical and safety related problems inherent in the process (batch or continuous). Alternatives that are more sustainable, compared to a reference, are generated and evaluated by addressing one or more of the identified problems. A decomposition technique as well as a set of batch indicators for batch operations has been developed and added to the methodology so that a wide range of processes that operate in continuous mode, in semi-continuous and/or in batch modes can be improved. The principal calculation steps of the methodology for applications to continuous and batch processes are described, highlighting the main differences between them. Through two case studies, the application of the methodology, to obtain sustainable design alternatives for batch plants, is highlighted.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern)
Pages: 2075-2090
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 33
Issue number: 12
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
Design of Continuous Processes for Organic-Synthesis Based Production of Active Pharmaceutical Ingredients - a Methodology

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre
Design of Feasible Blends of Gasoline and Biofuels using a Systematic Computer Aided Technique

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Department of Management Engineering, Universiti Teknologi Malaysia
Authors: Yunus, N. A. (Intern), Manan, Z. A. (Ekstern), Hashim, H. (Ekstern), Gani, R. (Intern)
Publication date: 2010

Design of Sustainable Processes: Systematic Generation & Evaluation of Alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Gani, R. (Intern), Matos, H. A. (Ekstern)
Pages: 267-272
Publication date: 2010

Design of sustainable processes: Systematic generation and evaluation of alternatives (Best Paper Award)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Gani, R. (Intern), Matos, H. (Ekstern)
Publication date: 2010

Development of a Systematic Synthesis/Design Methodology incorporating Process Intensification

General information
Development of a Systematic Synthesis/Design Methodology incorporating Process Intensification

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266270
Publication: Research › Poster – Annual report year: 2010

Editorial

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Venkatasubramanian, V. (Ekstern), Gani, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 34
Issue number: 10
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
F3 process design for fine chemical and Pharmaceutical transformations

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Muller, F. (Ekstern), Sanchez, R. R. (Ekstern), Wrate, T. (Ekstern), Davison, S. (Ekstern), Manipura, A. (Ekstern)
, Martin, E. B. (Ekstern), Montague, G. A. (Ekstern), Kraut, M. (Ekstern), Haas-Santo, K. (Ekstern), Forsberg, K. (Ekstern),
Rasmuson, A. C. (Ekstern), Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 270206
Publication: Research - peer-review › Journal article – Annual report year: 2010

Formulation design: managing the complexity through the Virtual Laboratory

General information
ICAS-PAT: A Software for Design, Analysis and Validation of PAT Systems

In chemicals based product manufacturing, as in pharmaceutical, food and agrochemical industries, efficient and consistent process monitoring and analysis systems (PAT systems) have a very important role. These PAT systems ensure that the chemicals based product is manufactured with the specified end product qualities. In an earlier article,
Singh et al. [Singh, R., Gernaey, K. V., Gani, R. (2009). Model-based computer-aided framework for design of process monitoring and analysis systems. Computers & Chemical Engineering, 33, 22–42] proposed the use of a systematic model and data based methodology to design appropriate PAT systems. This methodology has now been implemented into a systematic computer-aided framework to develop a software (ICAS-PAT) for design, validation and analysis of PAT systems. Two supporting tools needed by ICAS-PAT have also been developed: a knowledge base (consisting of process knowledge as well as knowledge on measurement methods and tools) and a generic model library (consisting of process operational models). Through a tablet manufacturing process example, the application of ICAS-PAT is illustrated, highlighting as well, the main features of the software.

**General information**

**State:** Published

**Organisations:** Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center

**Authors:** Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)

**Pages:** 1108-1136

**Publication date:** 2010

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

**Publication information**

**Journal:** Computers & Chemical Engineering

**Volume:** 34

**Issue number:** 7

**ISSN (Print):** 0098-1354

**Ratings:**

- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Web of Science (2016): Indexed yes
- Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Web of Science (2015): Indexed yes
- Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Web of Science (2014): Indexed yes
- Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Web of Science (2013): Indexed yes
- Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
- Web of Science (2012): Indexed yes
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.176 SNIP 1.796
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.154 SNIP 2.166
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 1.293 SNIP 2.127
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.625 SNIP 1.959
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.304 SNIP 1.936

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Roman Martinez, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Implementation 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
Authors: Abd.Hamid, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 683-699
Publication date: 2010
Main Research Area: Technical/natural sciences
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.293 SNIP 2.127
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.625 SNIP 1.959
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.304 SNIP 1.936
Scopus rating (2005): SJR 1.314 SNIP 1.953
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.125 SNIP 1.908
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.348 SNIP 1.936
Scopus rating (2002): SJR 1.042 SNIP 0.92
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.955 SNIP 0.728
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.366 SNIP 1.025
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.073 SNIP 1.113

Original language: English
DOIs:
10.1016/j.compchemeng.2010.01.016
Source: orbit
Source-ID: 250520
Publication: Research - peer-review › Journal article – Annual report year: 2010
Managing the Complexity in Liquid Formulation Design

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Gani, R. (Intern)
Publication date: 2010

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 268882
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Managing the complexity in product and process engineering

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 272677
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Managing the Complexity in Product and Process Engineering

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 268902
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Mechanistic modeling for systematic design and analysis of PAT systems (Invited Lecture)

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Singh, R. (Intern), Abdul Samad, N. A. F. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Methods and Tools to Overcome the Lack of Data in Property Prediction in Lipid Processing Technology

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Publication date: 2010

Model-based design and analysis of integrated biocatalytic processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Roman Martinez, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Number of pages: 135
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Main Research Area: Technical/natural sciences
Conference: 3. Dansk KemiingeniørKonference, Kgs. Lyngby, Denmark, 16/06/2010 - 16/06/2010
Source: orbit
Source-ID: 266247
Publication: Research › Article in proceedings – Annual report year: 2010

Model-based design and analysis of integrated biocatalytic processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Roman Martinez, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266274
Publication: Research › Poster – Annual report year: 2010

Model-based Design and Analysis of Integrated Biocatalytic Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Roman Martinez, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010
Moving from batch toward continuous organic-chemical pharmaceutical production

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre
Authors: Cervera Padrell, A. E. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Kiil, S. (Intern), Skovby, T. (Ekstern)
Pages: 133-134
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Main Research Area: Technical/natural sciences
Conference: 3. Dansk KemiingeniørKonference, Kgs. Lyngby, Denmark, 16/06/2010 - 16/06/2010
Source: orbit
Source-ID: 266234
Publication: Research › Article in proceedings – Annual report year: 2010

Moving from batch toward continuous organic-chemical pharmaceutical production

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre
Authors: Cervera Padrell, A. E. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Kiil, S. (Intern), Skovby, T. (Ekstern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266261
Publication: Research › Poster – Annual report year: 2010

Multiple steady states detection in a packed-bed reactive distillation column using bifurcation analysis
A packed reactive distillation column producing ethyl tert-butyl ether from tert-butyl alcohol and ethanol was simulated for detection of multiple steady states using Aspen Plus®. A rate-based approach was used to make the simulation model more realistic. A base-case was first developed and fine-tuned to fit experimental data. Sensitivity analyses were then performed for reboiler duty and distillate molar flow as continuation parameters to trace the respective bifurcation curves in the region of multiplicity. The results show output multiplicity at three distinct steady states at high reboiler duties. Input multiplicities were detected at high reflux ratios. Temperature and composition profiles of the solution branches were analyzed to identify the stable and desirable steady state. The optimum operating point was determined to be at a reboiler duty of 0.38 kW and a reflux ratio of 5–7. These results closely match the experimental results.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ramzan, N. (Ekstern), Faheem, M. (Ekstern), Gani, R. (Intern), Witt, W. (Ekstern)
Pages: 460-466
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 34
Issue number: 4
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Process Design for Chemo-enzymatic Synthesis of 2,5-Furandicarboxylic Acid

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Computer Aided Process Engineering Center
Authors: Fu, W. (Intern), Jensen, J. S. (Intern), Boisen, A. (Intern), Pedersen, S. (Ekstern), Riisager, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 268762
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Process Design for Chemo-enzymatic Synthesis of 2,5-Furandicarboxylic Acid (Best Poster Award)

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Computer Aided Process Engineering Center
Authors: Fu, W. (Intern), Jensen, J. S. (Intern), Boisen, A. (Ekstern), Pedersen, S. (Ekstern), Riisager, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265199
Publication: Research - peer-review › Poster – Annual report year: 2010

Process Design for chemo-enzymatic synthesis of 5-hydroxymethylfurfural

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Computer Aided Process Engineering Center
Authors: Fu, W. (Intern), Jensen, J. S. (Intern), Riisager, A. (Intern), Pedersen, S. (Ekstern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 267265
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Process Design for Chemo-enzymatic Synthesis of 5-Hydroxymethylfurfural

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Sustainable and Green Chemistry, Department of Chemistry, Computer Aided Process Engineering Center, Centre for Catalysis and Sustainable Chemistry
Number of pages: 205
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemingeniørkonference 2010
Main Research Area: Technical/natural sciences
Process Design for Chemo-enzymatic Synthesis of 5-Hydroxymethylfurfural

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Sustainable and Green Chemistry, Department of Chemistry, Computer Aided Process Engineering Center, Centre for Catalysis and Sustainable Chemistry
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266239
Publication: Research › Article in proceedings – Annual report year: 2010

Process Intensification: A Perspective on Process Synthesis
In recent years, process intensification (PI) has attracted considerable academic interest as a potential means for process improvement, to meet the increasing demands for sustainable production. A variety of intensified operations developed in academia and industry creates a large number of options to potentially improve the process but to identify the set of feasible solutions for PI in which the optimal can be found takes considerable resources. Hence, a process synthesis tool to achieve PI would potentially assist in the generation and evaluation of PI options. Currently, several process design tools with a clear focus on specific PI tasks exist. Therefore, in this paper, the concept of a general systematic framework for synthesis and design of PI options in hierarchical steps through analyzing an existing process, generating PI options in a superstructure and evaluating intensified process options is presented. For each step, different tools and methods will be needed. In this paper, a knowledge base tool storing and retrieving necessary information/data about intensified processes/equipments has been highlighted including metrics for performance evaluation. The application of the main concepts is illustrated through an example involving the operation of a membrane reactor.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Pages: 547-558
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266266
Publication: Research › Poster – Annual report year: 2010

Publication information
Journal: Chemical Engineering and Processing
Volume: 49
Issue number: 6
ISSN (Print): 0255-2701
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.766 SNP 1.205 CiteScore 2.57
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.837 SNP 1.389 CiteScore 2.63
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.87 SNP 1.427 CiteScore 2.41
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.972 SNP 1.391 CiteScore 2.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Property modeling for applications in chemical product and process design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265927
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Property Modelling for Applications in Chemical Product and Process Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265930
Property modelling for applications in product and process Engineering

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Property Prediction for Lipids Based Product Design and Analysis

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Publication date: 2010

Recent Advances in Reactive Distillation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern), Dada, E. A. (Ekstern)
Publication date: 2010

Recent Advances in Reactive Distillation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern), Dada, E. A. (Ekstern)
Publication date: 2010
Recent Advances in Reactive Distillation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern), Dada, E. A. (Ekstern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 272687
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Simulation of thin-film deodorizers in palm oil refining
As the need for healthier fats and oils (natural vitamin and trans fat contents) and interest in biofuels are growing, many changes in the world's vegetable oil market are driving the oil industry to developing new technologies and recycling traditional ones. Computational simulation is widely used in the chemical and petrochemical industries as a tool for optimization and design of (new) processes, but that is not the case for the edible oil industry. Thin-film deodorizers are novel equipment developed for steam deacidification of vegetable oils, and no work on the simulation of this type of equipment could be found in the open literature. This paper tries to fill this gap by presenting results from the study of the effect of processing variables, such as temperature, pressure and percentage of stripping steam, in the final quality of product (deacidified palm oil) in terms of final oil acidity, the tocopherol content and neutral oil loss. The simulation results have been evaluated by using the response surface methodology. The model generated by the statistical analysis for tocopherol retention has been validated by matching its results with industrial data published in the open literature.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, State University of Campinas
Authors: Ceriani, R. (Intern), Meirelles, A. J. (Ekstern), Gani, R. (Intern)
Pages: 208-225
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Food Process Engineering
Volume: 33
Issue number: suppl. 1
ISSN (Print): 0145-8876
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.15 SJR 0.471 SNIP 0.697
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.374 SNIP 0.7 CiteScore 0.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.424 SNIP 0.571 CiteScore 0.86
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.376 SNIP 0.76 CiteScore 0.84
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.336 SNIP 0.57 CiteScore 0.68
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.333 SNIP 0.466 CiteScore 0.71
Solvent Selection and Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229157
Publication: Research › Journal article – Annual report year: 2010

Solvents, green chemistry and sustainable product-process design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265924
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Matos, H. A. (Ekstern), Carvalho, A. I. C. D. S. G. (Ekstern)
Pages: 159-188
Publication date: 2010

Host publication information
Title of host publication: Managing CO2 Emissions in the Chemical Industry : Chapter 5
Editor: Leimkühler, H.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 256597
Publication: Research - peer-review › Book chapter – Annual report year: 2010

Sustainable design for an olefin process (Best Poster Award)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: N. Iyara, N. I. (Ekstern), Siemanond, K. (Ekstern), Gani, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265201
Publication: Research - peer-review › Poster – Annual report year: 2010

Sustainable design of chemical and bio-chemical processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 272681
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Sustainable process design for lignocellulosic-based bioethanol using life cycle assessment technique

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Tansutapanich, P. (Ekstern), Malakul, P. (Ekstern), Gani, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265202
Publication: Research - peer-review › Poster – Annual report year: 2010

Synthesis, Design and Analysis of Downstream Separation in Bio-refinery Processes through a Group- Contribution Approach

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Computer Aided Process Engineering Center
Systematic computer-aided method and tool (ICAS-PAT) for design, analysis &/or validation of process monitoring and analysis systems (PAT systems)

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 267041
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Systematic Design of An Acetaldehyde Process

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Babi, D. K. (Intern), Price, J. A. (Intern), Gani, R. (Intern)
Publication date: 2010
Event: Poster session presented at 2010 AIChE Annual Meeting, Salt Lake City, United States.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 268900
Publication: Research - peer-review › Poster – Annual report year: 2010

Systematic Framework for Design and Adaption of Fast, Flexible, Continuous Modular Plants

General information
State: Published
Systematic method and tool for design, analysis &/or validation of PAT systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2010

Systematic methodology and property prediction of fatty systems for process design/analysis in the oil and fat industry

A systematic model based methodology has been developed and its application highlighted through the solvent recovery section of a soybean oil extraction process, with emphasis on the effect of design variables on the process performance. First, the most representative compounds present in the vegetable oil were defined. Basic and critical properties were then computed by means of appropriate property prediction software. Temperature dependant properties were modeled using and extending available correlations. The process model was developed through the PRO II commercial simulator and validated by matching the steady state simulation results with available plant data. The validated process model was then used to optimize the performance of the process by manipulating a selected set of design variables. The optimization results indicated that the process was already within the optimum zone; however, improvements in the amount of the hexane recovered were possible.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Ceriani, R. (Ekstern), Gani, R. (Intern), Sarup, B. (Ekstern)
Pages: 401-412
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Brazilian Journal of Chemical Engineering
Volume: 27
Issue number: 3
ISSN (Print): 0104-6632
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.429 SNIP 0.965 CiteScore 1.46
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.426 SNIP 0.967 CiteScore 1.29
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.411 SNIP 0.851 CiteScore 1.3
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.449 SNIP 0.91 CiteScore 1.26
The calculation of thermodynamic properties of molecules

Thermodynamic data are key in the understanding and design of chemical processes. Next to the experimental evaluation of such data, computational methods are valuable and sometimes indispensable tools in obtaining heats of formation and Gibbs free energies. The major toolboxes to obtain such quantities by computation are quantum mechanical methods and group contribution methods. Although a lot of progress was made over the last decade, for the majority of chemical species we are still quite a bit away from what is often referred to as chemical accuracy, i.e. 1 kcal mol⁻¹. Currently, for larger molecules the combination of group contribution methods with group additive values that are determined with the best available computational ab initio methods seems to be a viable alternative to obtain thermodynamic properties near chemical accuracy. New developments and full use of existing tools may lead to further improvements.
Thermodynamics – our molecular sister or just a forgotten relative? (Invited Lecture)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
The Virtual Product-Process Design Laboratory applied to personal care formulations

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Gani, R. (Intern), Malik, T. (Ekstern)
Pages: 1297-1302
Publication date: 2010

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 28
Publisher: Elsevier Science
Main Research Area: Technical/natural sciences
Conference: 20th European Symposium on Computer Aided Process Engineering, Ischia, Italy, 06/06/2010 - 06/06/2010
Source-ID: 255448
Publication: Research - peer-review » Article in proceedings – Annual report year: 2010

The Virtual Product-Process Design Laboratory to Manage the Complexity in Formulation Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Gani, R. (Intern), Malik, T. I. (Ekstern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source-ID: 265208
Publication: Research » Sound/Visual production (digital) – Annual report year: 2010

The Virtual Product-Process Laboratory applied to personal care formulations

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Gani, R. (Intern), Malik, T. (Ekstern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source-ID: 265225
Publication: Research » Sound/Visual production (digital) – Annual report year: 2010

Towards the Merging of Property Prediction & Process Design/Analysis in the Edible Oil Industry

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Publication date: 2010
Event: Poster session presented at CAPE Forum 2010, Aachen, Germany.
Main Research Area: Technical/natural sciences
Source-ID: 265116

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gani, R. (Intern), Gernaey, K. (Intern)
Publication date: Nov 2009

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Ravendra Singh_PEC09-47.pdf
Source: orbit
Source-ID: 252281
Publication: Research › Ph.D. thesis – Annual report year: 2009

Model-based retrofit design and analysis of petrochemical processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Rashed, J. E. A. (Intern), Gani, R. (Intern)
Number of pages: 123
Publication date: Nov 2009

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 252280
Publication: Research › Ph.D. thesis – Annual report year: 2009

Computer-aided polymer design using Multiscale modeling

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Chelakara Satyanarayana, K. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Number of pages: 256
Publication date: Sep 2009

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 252279
Publication: Research › Ph.D. thesis – Annual report year: 2009

Computer-Aided Multiscale Modelling for Chemical Product-Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Development of Group Contributionplus Models for Properties of Organic Chemical Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Gani, R. (Intern), Abildskov, J. (Intern)
Publication date: Aug 2009

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
Authors: Heitzig, M. (Intern), Sin, G. (Intern), Glarborg, P. (Intern), Gani, R. (Intern)
Publication date: 2009

A Computer-Aided Tool for Applying the Multiscale Modeling Needs In Innovative Product-Process Engineering

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Heitzig, M. (Intern), Morales Rodriguez, R. (Intern), Sin, G. (Intern), Glarborg, P. (Intern), Gani, R. (Intern)
Publication date: 2009
A general model for membrane-based separation processes

A separation process could be defined as a process that transforms a given mixture of chemicals into two or more compositionally distinct end-use products. One way to design these separation processes is to employ a model-based approach, where mathematical models that reliably predict the process behaviour will play an important role. In this paper, modelling of membrane-based processes for separation of gas and liquid mixtures are considered. Two general models, one for membrane-based liquid separation processes (with phase change) and another for membrane-based gas separation are presented. The separation processes covered are: membrane-based gas separation processes, pervaporation and various types of membrane distillation processes. The specific model for each type of membrane-based process is generated from the two general models by applying the specific system descriptions and the corresponding modelling assumptions. Analyses of the generated models, together with their validation and application in process design/analysis are highlighted through several case studies.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Pages: 644-659
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 33
Issue number: 3
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.293 SNIP 2.127
A Group Contribution Method for Mineral Flotation Circuit Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gálvez, E. D. (Ekstern), Cisternas, L. A. (Ekstern), Herrera, G. (Ekstern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248618
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

A Group Contribution Method for Mineral Flotation Circuit Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gálvez, E. D. (Ekstern), Cisternas, L. A. (Ekstern), Herrera, G. (Ekstern), Gani, R. (Intern)
Number of pages: 1,224
Publication date: 2009

Host publication information
Title of host publication: Proceedings of 10th International Symposium on Process Systems Engineering
Publisher: Elsevier Science
Editors: Brito Alves, R. M. D., Nascimento, C. A. O. D., Chalbaud Biscia Jr., E.
ISBN (Print): 9780444534354

Series: Computer - Aided Chemical Engineering
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 250903
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009
Analysis of a Concept for Predicting Missing Group Interaction Parameters of the UNIFAC Model Using Connectivity Indices

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Gonzalez Villalba, H. E. (Intern)
Pages: 1626-1627
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: AIChE Journal
Volume: 55
Issue number: 6
ISSN (Print): 0001-1541
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.004 SNIP 1.234 CiteScore 2.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.083 SNIP 1.423
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.192 SNIP 1.437
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.287 SNIP 1.428
A new model-based methodology for simultaneous design and control of reaction-separation systems with recycle

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Abd.Hamid, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248310
Publication: Research - peer-review › Journal article – Annual report year: 2009

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

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Abd.Hamid, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 839-845
Publication date: 2009

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 26
Publisher: Elsevier
Main Research Area: Technical/natural sciences
Conference: 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14/06/2009 - 14/06/2009
Source: orbit
Source-ID: 231828
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009
Application of ICAS-PAT On Design of Process Monitoring and Control System for a Batch Cooling Crystallization Process through Hybrid Multiscale Model-Based Analysis

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Abdul Samad, N. A. F. (Intern), Singh, R. (Intern), Sin, G. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 252823
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Application of the GC-plus approach to PC-SAFT EOS and prediction of phase Equilibria

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Privat, R. (Intern), Gani, R. (Intern), Jaubert, J. (Ekstern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248259
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Application of the GC-plus approach to PC-SAFT EOS and prediction of phase Equilibria

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Privat, R. (Intern), Gani, R. (Intern), Jaubert, J. (Ekstern)
Number of pages: 73
Publication date: 2009

Host publication information
Title of host publication: Proceedings of the 24th European Symposium on Applied Thermodynamics, Edited by: Alberto Arce and Ana Soto
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248265
Publication: Research › Article in proceedings – Annual report year: 2009

A Process Systems Engineering Approach for Managing the Complexity in Chemical Product-Process Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
A software tool for design of process monitoring and analysis systems

A well designed process monitoring and analysis system is necessary to consistently achieve any predefined end product quality. Systematic computer aided methods and tools provide the means to design the necessary process monitoring and analysis systems and/or to validate any existing monitoring and analysis system. A software to achieve this has been developed. Two developed supporting tools for the design, a knowledge base (consisting of the process knowledge as well as the knowledge on measurement methods & tools) and a model library (consisting of the process operational models) have been extended rigorously and integrated with the user interface, which made the software more generic and applicable to a wide range of problems. The software for the design of a process monitoring and analysis system is presented and illustrated with a tablet manufacturing process example.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Pages: 321-326
Publication date: 2009

A systematic computer aided framework for design and analysis of PAT systems

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gernaey, K. (Intern), Singh, R. (Intern), Gani, R. (Intern)
Publication date: 2009

A Systematic Methodology to Synthesize and Design Processes, Incorporating Process Intensification

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lutze, P. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2009
A Systems Approach for Design of Intensified Bio-Pharmaceutical Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Román-Martinez, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2009

Biodiesel Process Design through a Computer-aided Molecular Design Approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Karunanithi, A. T. (Ekstern), Gani, R. (Intern), Achenie, L. E. (Ekstern)
Publication date: 2009

Biorefining: Computer aided tools for sustainable design and analysis of bioethanol production

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Computer Aided Process Engineering Center
Authors: Alvarado-Morales, M. (Intern), Terra, J. (Ekstern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Pages: 1171-1183
Computer aided design, analysis and experimental investigation of membrane assisted batch reaction-separation systems

Membrane assisted batch reaction operation offers an interesting option for equilibrium limited reaction systems in chemical and biochemical manufacturing by selective removal of one of the products and thereby increasing the product yield. The design of such hybrid systems need to take into account the performance of each constituent element and the optimisation of the design must take into consideration their interdependency. In this paper use of a membrane, to assist in the synthesis of propyl-propionate is investigated through the use of a hybrid process design framework, which consists of a process design/analysis stage, a process implementation stage and a process verification stage. For the hybrid process design/analysis stage, a model-based methodology has been developed and integrated with the necessary computer-aided methods/tools to identify the operational window of reaction and separation functionalities and to design/analyse the hybrid scheme. The generated hybrid scheme has been validated through experiments involving an esterification reaction.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mitkowski, P. T. (Intern), Buchaly, C. (Ekstern), Kreis, P. (Ekstern), Jonsson, G. E. (Intern), Gorak, A. (Ekstern), Gani, R. (Intern)
Computer-aided polymer design using group contribution plus property models
The preliminary step for polymer product design is to identify the basic repeat unit structure of the polymer that matches the target properties. Computer-aided molecular design (CAMD) approaches can be applied for generating the polymer repeat unit structures that match the required constraints. Polymer repeat unit property prediction models are required to calculate the properties of the generated repeat units. A systematic framework incorporating recently developed group contribution plus (GC(+)) models and an extended CAMD technique to include design of polymer repeat units is highlighted in this paper. The advantage of a GC(+) model in CAMD applications is that a very large number of polymer structures can be considered even though some of the group parameters may not be available. A number of case studies involving different polymer design problems have been solved through the developed framework. The paper highlights three such case studies.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Pages: 1004-1013
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 33
Issue number: 5
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.293 SNIP 2.127
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.625 SNIP 1.959
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.304 SNIP 1.936
Scopus rating (2005): SJR 1.314 SNIP 1.953
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.125 SNIP 1.908
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.348 SNIP 1.936
Scopus rating (2002): SJR 1.042 SNIP 0.92
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.955 SNIP 0.728
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.366 SNIP 1.025
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.073 SNIP 1.113
Original language: English
Polymer property, Group contributions plus, CAMD, Property model
DOIs:
10.1016/j.compchemeng.2008.09.021
Source: orbit
Source-ID: 243151
Publication: Research - peer-review › Journal article – Annual report year: 2009

**Computer aided polymer design using multiscale modelling**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2009

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 255460
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

**Computers & Chemical Engineering: Best paper of 2007**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Pages: 1905-1906
Publication date: 2009
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Computers & Chemical Engineering
Volume: 33
Design methodology for intensified bioprocesses

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Román-Martinez, A. (Intern), Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248166
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Design of Sustainable Chemical Processes: Systematic Retrofit Analysis Generation and Evaluation of Alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. I. C. D. S. G. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern)
Publication date: 2009

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Ana Carvalho_PEC09-62.pdf
Source: orbit
Source-ID: 255282
Publication: Research › Ph.D. thesis – Annual report year: 2009

Design Strategies for Neuraminic Acid Synthesis: Comparative Study of Chemical and Biochemical Routes and Integration of Purification Steps

General information
State: Published
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
Authors: Abd.Hamid, M. (Intern), Sin, G. (Intern), Gani, R. (Intern)
Pages: 593-602
Publication date: 2009

Host publication information
Title of host publication: Proceedings for FOCAPD-2009
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 231830
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Direct Calculation of PC-SAFT Parameters From Experimental LVE Data and From a GC-Plus Approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Privat, R. (Intern), Gani, R. (Intern), Jaubert, J. (Ekstern)
Publication date: 2009
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 252827
Publication: Research - peer-review › Poster – Annual report year: 2009

Editorial note
The “aims and scope” of the Computers & Chemical Engineering has been revised (see the inside cover page for the new version). We would like to make this journal the indisputable journal for the Process Systems Engineering (PSE) area as well as define the PSE agenda for the future. The principal components of PSE—modeling, numerical analysis, optimization, systems and control theory, computer science, and, management science will be highlighted through the published articles (full-length papers, perspective papers, review papers, short notes and letters to the editor). They will cover the traditional areas in PSE together with the emerging challenges in PSE in terms of: PSE core methodologies...
(numerical analysis, optimization methods, etc.), PSE core domains (modeling, synthesis/design, control, operation, monitoring, etc.); PSE emerging methodologies (cyberinfrastructure, informatics and intelligent systems, integrated approaches to design, control and data analysis, systematic techniques for managing complexity, etc.), PSE emerging domains (product-process design, enterprise-wide optimization, energy and sustainability, biological engineering, pharmaceutical engineering, etc.) and novel industrial and educational applications. These articles will highlight theory, models, algorithms and applications with respect to value preservation and/or value creation or growth within the chemical product supply chain. To highlight and motivate research in the emerging challenges in PSE, we plan to publish three or four perspective papers per year on selected topics. The following perspective papers on the following topics are planned for 2009: "bioprocess modeling and evaluation"; "support systems for design, management and implementation of policies" and "molecular products design and engineering". Readers are welcome to suggest topics for future perspective papers.

We will try our best to bring down the processing time of submitted manuscripts. We hope to provide authors with the first stage decision and reviewer comments within three to six months after submission of their manuscript. Here, we need your support and cooperation as potential reviewers. We would very much appreciate if reviewers, who accept our invitation to review, send their comments to us within the agreed deadline. We will strive to maintain and strengthen the scientific quality of Computers & Chemical Engineering and make it one of the leading journals within Chemical Engineering and beyond with a wide audience. To introduce the new theme of "Cyberinfrastructure, informatics, and intelligent systems" a short commentary on this topic is included in this issue of Computers & Chemical Engineering.

Finally, we would like to thank Professor Rex Reklaitis for leading this journal for 22 years and making it one of the leading journals within Chemical Engineering.

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Authors: Gani, R. (Intern), Hrymak, A. (Ekstern), Lee, J. (Ekstern), Venkatasubramanian, V. (Ekstern)
Pages: 1-1
Publication date: 2009
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Computers & Chemical Engineering
Volume: 33
Issue number: 1
ISSN (Print): 0098-1354
Ratings:
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.176 SNIP 1.796
GC, GC+ (Group Contribution Plus) and Atom Connectivity Index-Based Models for Physical Properties of Lipid Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ceriani, R. (Intern), Conte, E. (Intern), Ellegaard, M. D. (Intern), Díaz Tovar, C. A. (Intern), Gonçalves, C. B. (Ekstern), Meirelles, A. J. (Ekstern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248260
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

GC, GC+ (Group Contribution Plus) and Atom Connectivity Index-Based Models for Physical Properties of Lipid Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ceriani, R. (Intern), Conte, E. (Intern), Ellegaard, M. D. (Intern), Díaz Tovar, C. A. (Intern), Gonçalves, C. B. (Ekstern), Meirelles, A. J. (Ekstern), Gani, R. (Intern)
Pages: 20-21
Publication date: 2009

Host publication information
Title of host publication: Proceedings of the 24th European Symposium on Applied Thermodynamics, Edited by: Alberto Arce and Ana Soto
Main Research Area: Technical/natural sciences
ICAS-PAT: A new software tool for systematic design/validation of process monitoring and analysis systems (PAT systems)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248266
Publication: Research › Article in proceedings – Annual report year: 2009

Integrated design of solvent based extractive separation processes including experimental validation

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Lek-utaiwan, P. (Ekstern), Suphanit, B. (Ekstern), Mongkolsiri, N. (Ekstern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248162
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Integrated design of solvent based extractive separation processes including experimental validation

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Lek-utaiwan, P. (Ekstern), Puphnit, B. (Ekstern), Mongkolsiri, N. (Ekstern), Gani, R. (Intern)
Pages: 201-206
Publication date: 2009

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 26
Publisher: Elsevier
Main Research Area: Technical/natural sciences
Conference: 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14/06/2009 - 14/06/2009
Source: orbit
Source-ID: 231790
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

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
Managing the complexity in product-process design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248163
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Managing the complexity in product-process design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Pages: 5-6
Publication date: 2009

Host publication information
Title of host publication: Proceedings of AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingeniería Química 2009)
Main Research Area: Technical/natural sciences
Conference: Academia Mexicana de Investigación y Docencia en Ingeniería Química, Mazatlan, Mexico, 19/05/2009 - 19/05/2009
Source: orbit
Source-ID: 248230
Publication: Research › Article in proceedings – Annual report year: 2009

Model-based Computer Aided Framework for Design of Process Monitoring and Analysis Systems
In the manufacturing industry, for example, the pharmaceutical industry, a thorough understanding of the process is necessary in addition to a properly designed monitoring and analysis system (PAT system) to consistently obtain the desired end-product properties. A model-based computer-aided framework including the methods and tools through which the design of monitoring and analysis systems for product quality control can be generated, analyzed and/or validated, has been developed. Two important supporting tools developed as part of the framework are a knowledge base and a model library. The knowledge base provides the necessary information/data during the design of the PAT system while the model
library generates additional or missing data needed for design and analysis. Optimization of the PAT system design is achieved in terms of product data analysis time and/or cost of monitoring equipment subject to the maintenance constraints of the desired product quality. The application of the model-based framework is highlighted through a case study involving the operation of a fermentation process.

**General information**

**State:** Published

**Organisations:** Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering

**Authors:** Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)

**Pages:** 22-42

**Publication date:** 2009

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

**Publication information**

**Journal:** Computers & Chemical Engineering

**Volume:** 33

**Issue number:** 1

**ISSN (Print):** 0098-1354

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- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.176 SNIP 1.796
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.154 SNIP 2.166
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 1.293 SNIP 2.127
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.625 SNIP 1.959
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.304 SNIP 1.936
- Scopus rating (2005): SJR 1.314 SNIP 1.953
- Web of Science (2005): Indexed yes
Model-based retrofit design and analysis of petrochemical processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Rashed, J. E. A. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248154
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Host publication information
Title of host publication: Proceedings of 1st Annual Gas Processing Symposium
Volume: 1
Publisher: Elsevier Science
ISBN (Print): 04-44-53292-7
Main Research Area: Technical/natural sciences
Conference: 1st Annual Gas Processing Symposium, Doha, Qatar, 10/01/2009 - 10/01/2009
Links:
http://www.worldcat.org/oclc/246896164
Source: orbit
Source-ID: 248227
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009
Model-based retrofit design and analysis of petrochemical processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Rashed, J. E. A. (Intern), Gani, R. (Intern)
Pages: 105-110
Publication date: 2009

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 26
Publisher: Elsevier
Main Research Area: Technical/natural sciences
Conference: 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14/06/2009 - 14/06/2009
Source: orbit
Source-ID: 231789
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Modelling for PSE and Product-Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248300
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Modelling for PSE and Product-Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Pages: 7-12
Publication date: 2009

Host publication information
Volume: 27A
Editors: Alves, R. M. D. B., Oller do Nascimento, C. A., Chalbaud Biscia Jr., E.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248549
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009
Multiscale Modelling Framework for Chemical Product-Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248202
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Multiscale Modelling Framework for Chemical Product-Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Pages: 495-500
Publication date: 2009

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 26
Publisher: Elsevier
Main Research Area: Technical/natural sciences
Conference: 19th European Symposium on Computer Aided Process Engineering – ESCAPE19, Krakow, Poland, 14/06/2009 - 14/06/2009
Source: orbit
Source-ID: 231389
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Optimization of long-term planning, supply chain and processing routes for tailor-made bio-chemicals

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Operations Management, Department of Management Engineering, CHEC Research Centre
Authors: Swangkotchakorn, C. (Intern), Hansen, K. R. N. (Intern), Grunwaldt, J. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265098
Publication: Research - peer-review › Report – Annual report year: 2009

Optimization of tailor-made chemicals from renewable and non-renewable sources

General information
State: Published
PC-SAFT equation of state: easy determination of model parameters and their use for prediction of pure component and mixture properties
Prediction of heat capacities and heats of vaporization of organic liquids by group contribution methods

In the present work a group contribution method is proposed for the estimation of the heat capacity of organic liquids as a function of temperature for fatty compounds found in edible oil and biofuels industries. The data bank used for regression of the group contribution parameters (1395 values for 86 types of substances) included fatty compounds, such as fatty acids, esters, alcohols and triacylglycerols, and hydrocarbons. The performance of this method is compared with other published group contribution methods [Z. Kolska, J. Kukal, M. Zabransky, V. Ruzicka Ind. Eng. Chem. Res. 47 (2008) 2075-2085] and the Rowlinson-Bondi equation. Also, the predictive performance of general correlations of heats of vaporization based on the corresponding-states method, such as Carruth and Kobayashi [G.F. Carruth, R. Kobayashi, Ind. Eng. Chem. Fundam. 11 (1972) 509-516], Sivaraman et al. [A. Sivaraman, J.W. Magee, R. Kobayashi, Ind. Eng. Chem. Fundam. 23 (1984) 97-100], and Morgan and Kobayashi [D.L. Morgan, R. Kobayashi, Fluid Phase Equilib. 121 (1996) 51-65], have been studied for fatty compounds. An alternative method in the prediction of heats of vaporization of fatty compounds based on the vapor pressure model of Ceriani and Meirelles [R. Ceriani. A.J.A. Meirelles, Fluid Phase Equilib. 215 (2004) 227-236] and its combination with the Clausius-Clapeyron equation has been studied. (C) 2009 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ceriani, R. (Intern), Gani, R. (Intern), Meirelles, A. (Ekstern)
Pages: 49-55
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 283
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Privat, R. (Intern), Gani, R. (Intern), Jaubert, J. (Ekstern)
Publication date: 2009
Process design and production of chemicals. Food ingredients, fuels and pharmaceuticals

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Meyer, A. S. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Pages: 170-179
Publication date: 2009

Host publication information
Title of host publication: Engineering challenges: energy, climate change and health
Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Editor: Hansen, C. B.
ISBN (Print): 978-87-985544-4-8
Series: DTU research series
Main Research Area: Technical/natural sciences
Electronic versions:
Engineering_challenges_2009.pdf
Source: orbit
Source-ID: 255723
Publication: Research › Book chapter – Annual report year: 2009

Product-Process Design Multiscale Modelling Framework

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248169
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Product-Process Design Multiscale Modelling Framework

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Number of pages: 286
Publication date: 2009

Host publication information
Title of host publication: Proceedings of AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingeniería Química 2009)
Main Research Area: Technical/natural sciences
Conference: Academia Mexicana de Investigación y Docencia en Ingeniería Química, Mazatlan, Mexico, 19/05/2009 - 19/05/2009
Source: orbit
Source-ID: 248223
Property modeling for applications in chemical product and process design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 255462
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Simulation and Optimization of a Solvent Recovery Process in the Vegetable Oil Industry

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Ceriani, R. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248164
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Simulation and Optimization of a Solvent Recovery Process in the Vegetable Oil Industry

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Ceriani, R. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Number of pages: 287
Publication date: 2009

Host publication information
Title of host publication: Proceedings of AMIDIQ XXX (Academia Mexicana de Investigación y Docencia en Ingeniería Química 2009)
Main Research Area: Technical/natural sciences
Conference: Academia Mexicana de Investigación y Docencia en Ingeniería Química, Mazatlan, Mexico, 19/05/2009 - 19/05/2009
Source: orbit
Source-ID: 248231
Publication: Research › Article in proceedings – Annual report year: 2009

Solvent selection and design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Special issue on "Chemical products: from conceptualization to commercialization" Preface

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ng, K. (Ekstern), Gani, R. (Intern), Seider, W. D. (Ekstern)
Pages: 929-929
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 33
Issue number: 5
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.293 SNIP 2.127
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.625 SNIP 1.959
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.304 SNIP 1.936
Scopus rating (2005): SJR 1.314 SNIP 1.953
Web of Science (2005): Indexed yes
Sustainability Analysis of Chemical Processes Plants Using a Hybrid Heuristic and Indicator Model

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern)
Publication date: 2009

Publication Information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248305
Publication: Research - Sound/Visual production (digital) – Annual report year: 2009

Sustainability Analysis of Chemical Processes Plants Using a Hybrid Heuristic and Indicator Model

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Carvalho, A. (Ekstern), Halim, I. (Intern), Srinivasan, R. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern)
Pages: 837-842
Publication date: 2009

Host publication information
Volume: 27A
Publisher: Elsevier Science
Editors: Alves, R. M. D. B., Oller do Nascimento, C. A., Chalbaud Biscia Jr., E.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248550
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Sustainable Bioprocess Synthesis Routes for Tailor-Made Chemicals

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, CHEC Research Centre
Authors: Swangkotchakorn, C. (Intern), Gani, R. (Intern), Woodley, J. (Intern), Grunwaldt, J. (Intern)
Sustainable Design of Chemical and Biochemical Processes: The Role of Models and Modeling

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2009

Sustainable product centric process design (Keynote Lecture)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2009

Synthesis, Design and Analysis of Downstream Separation in Chemical and Bio-Processes

General information
State: Published
Organisations: Department of Environmental Engineering, Residual Resource Engineering, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Alvarado-Morales, M. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2009

Systematic Representation and Property Prediction of Fatty Systems for Process Design/Analysis in the Oil and Fat Industry

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Ceriani, R. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Systematic Representation and Property Prediction of Fatty Systems for Process Design/Analysis in the Oil and Fat Industry

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Díaz Tovar, C. A. (Intern), Ceriani, R. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Pages: 819-824
Publication date: 2009

Host publication information
Volume: 27A
Publisher: Elsevier Science
Editors: Alves, R. M. D. B., Oller do Nascimento, C. A., Chalbaud Biscia Jr., E.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248552
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Thermodynamic Property Modeling for Chemical Process and Product Engineering: Some Perspectives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: O’Connell, J. P. (Ekstern), Gani, R. (Intern), Mathias, P. M. (Ekstern), Maurer, G. (Ekstern), Olson, J. D. (Ekstern), Crafts, P. A. (Ekstern)
Pages: 4619-4637
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 48
Issue number: 10
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
The virtual Product-Process Design laboratory as a tool for product development

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Pages: 249-254
Publication date: 2009

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: 26
Publisher: Elsevier
The Virtual Product-Process Design Laboratory as a Tool for Product Development

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 231395
Publication: Research › Article in proceedings – Annual report year: 2009

The Virtual Product-Process Design Laboratory for Design and Analysis of Formulations

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248210
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Host publication information
Volume: 27A
Editors: Alves, R. M. D. B., Oller do Nascimento, C. A., Chalbaud Biscia Jr., E.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248545
Publication: Research › peer-review › Article in proceedings – Annual report year: 2009

The Virtual Product-Process Design Laboratory for the Design and Analysis of Formulations

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Conte, E. (Intern), Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 248298
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

The Virtual Product-Process Design Laboratory for the Design of Formulated Products

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

The Virtual Product-Process Design Laboratory as a Tool for Product Development
Computer aided design and analysis of reaction-separation and separation-separation systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mitkowski, P. T. (Intern), Gani, R. (Intern), Jonsson, G. E. (Intern)
Number of pages: 252
Publication date: Dec 2008

A Systematic Synthesis Framework for Extractive Distillation Processes

An effective extractive distillation process depends on the choice of the extractive agent. In this contribution, heuristic rules for entrainer selection and the design of entrainers through computer-aided molecular design are reviewed. The potential of the generated alternatives is then evaluated by their selectivity at infinite dilution and by the rectification body method (RBM). It is shown that a screening based on selectivity alone is not sufficient and could possibly lead to an unfavorable entrainer choice. The minimum entrainer flowrate and the minimum energy demand, calculated from the RBM, allow a more comprehensive evaluation of different entrainer alternatives. In a third step a rigorous mixed-integer optimization of the entire extractive flowsheet for the remaining entrainer candidates is executed to fix the remaining design degrees of freedom and to determine the best entrainer. Since a number of alternative entrainers have already been eliminated, only a few optimizations are necessary. These steps form a framework which facilitates the systematic generation and evaluation of entrainer alternatives. The suggested synthesis framework is illustrated with a case study where acetone and methanol are to be separated. (C) 2008 The Institution of Chemical Engineers. Published by Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Kossack, S. (Ekstern), Kraemer, K. (Ekstern), Gani, R. (Intern), Marquardt, W. (Ekstern)
Pages: 781-792
Publication date: Jul 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Research & Design
Volume: 86
Issue number: 7A
ISSN (Print): 0263-8762
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.855 SNIP 1.449 CiteScore 2.7
Chemically Structured Products: Simultaneous model-based design of process and assisting structured materials

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Soni, V. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Abildskov, J. (Intern)
Publication date: Jun 2008

Publication information
Original language: English
A model-based framework for design and analysis of PAT systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Gani, R. (Intern), Singh, R. (Intern), Gernaey, K. (Intern)
Publication date: 2008

A Model-Based Framework for Systematic Product Quality Monitoring and Control

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2008

A model-based methodology for simultaneous process design and control for chemical processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abd.Hamid, M. (Intern), Gani, R. (Intern)
Publication date: 2008

A Model-Based Systems Approach for Integrated Chemical Product-Process Design

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

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 221887
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

A process systems engineering approach for managing the complexity

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 231446
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

A Software Tool for Design of Process Monitoring and Analysis Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2008
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229270
Publication: Research - peer-review › Poster – Annual report year: 2008

A Systematic Methodology for the Selection of Green and Non-Reactive Solvents for Multistage Organic Reactions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Shafique Bashir, M. (Intern), Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
A Systematic Multiscale Modelling Framework for Product-Process Design and Development

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229329
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Atomistic Simulation of the Diffusion of Small Gas Molecules in Polyisobutylene

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Abildskov, J. (Intern), Gani, R. (Intern), Tsolou, G. (Ekstern), Mavrantzas, V. (Ekstern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229279
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Atomistic Simulation of the sorption of small gas molecules in polyisobutylene

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mavrantzas, V. (Ekstern), Tsolou, G. (Ekstern), Economou, I. (Ekstern), Makrodimitrie, Z. (Ekstern), Gani, R. (Intern)
Pages: 6228-6238
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Macromolecules
Volume: 41
Issue number: 16
ISSN (Print): 0024-9297
Ratings:
  BFI (2017): BFI-level 2
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 5.76 SJR 2.557 SNIP 1.507
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): SJR 2.407 SNIP 1.638 CiteScore 5.82
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 2.534 SNIP 1.721 CiteScore 5.83
Bioprocess Synthesis, Design and Analysis through a Group-Contribution Approach

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Computer Aided Process Engineering Center
Authors: Alvarado-Morales, M. (Intern), Terra, J. (Ekstern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Publication date: 2008

Publication information
Biorefinery: Analysis of Process Design Alternatives

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Al-Haque, N. (Intern), Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229336
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

CAPEC Research Report 2008

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Abildskov, J. (Intern)
Publication date: 2008

Publication information
Publisher: CAPEC-DTU
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 221008
Publication: Research › Report – Annual report year: 2008

CAPE methods and tools for systematic analysis of new chemical product design and development

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Computer Aided Process Engineering Center
Authors: Alvarado-Morales, M. (Intern), Al-Haque, N. (Intern), Gernaey, K. (Intern), Woodley, J. (Intern), Gani, R. (Intern)
Pages: 997-1002
Publication date: 2008

Host publication information
Title of host publication: Computer Aided Chemical Engineering, on CD
Volume: 25
Main Research Area: Technical/natural sciences
Conference: 18th European Symposium on Computer Aided Process Engineering , Lyon, France, 01/06/2008 - 01/06/2008
Source: orbit
Source-ID: 245184
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

Combined group-contribution and atom connectivity index based methods for estimation of surface tension and viscosity

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

Design of sustainable chemical processes: Systematic retrofit analysis, generation and evaluation alternatives

The objective of this paper is to present a generic and systematic methodology for identifying the feasible retrofit design alternatives of any chemical process. The methodology determines a set of mass and energy indicators from steady-state process data, establishes the operational and design targets, and through a sensitivity-based analysis, identifies the design alternatives that can match a set of design targets. The significance of this indicator-based method is that it is able
to identify alternatives, where one or more performance criteria (factors) move in the same direction thereby eliminating the need to identify trade-off-based solutions. These indicators are also able to reduce (where feasible) a set of safety indicators. An indicator sensitivity analysis algorithm has been added to the methodology to define design targets and to generate sustainable process alternatives. A computer-aided tool has been developed to facilitate the calculations needed for the application of the methodology. The application of the indicator-based methodology and the developed software are highlighted through a process flowsheet for the production of vinyl chlorine monomer (VCM).

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Gani, R. (Intern), Matos, H. (Ekstern)
Pages: 328-346
Publication date: 2008
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Process Safety and Environmental Protection
Volume: 86
Issue number: 5
ISSN (Print): 0957-5820
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3 SJR 0.685 SNIP 1.642
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.662 SNIP 1.352 CiteScore 2.55
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.078 SNIP 2.118 CiteScore 2.85
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.919 SNIP 1.869 CiteScore 2.22
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.763 SNIP 1.248 CiteScore 1.67
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.713 SNIP 1.205 CiteScore 1.65
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.825 SNIP 1.119
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.67 SNIP 0.782
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.296 SNIP 0.449
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.344 SNIP 0.907
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.411 SNIP 0.763
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.404 SNIP 0.738
Scopus rating (2004): SJR 0.403 SNIP 0.584
Scopus rating (2003): SJR 0.583 SNIP 1.125
Scopus rating (2002): SJR 0.599 SNIP 0.897
Scopus rating (2001): SJR 0.31 SNIP 0.863
Scopus rating (2000): SJR 0.666 SNIP 0.938
Scopus rating (1999): SJR 0.382 SNIP 0.773
Original language: English

DOIs:
Design of Sustainable Chemical Process: Systematic Retrofit Analysis Generation and Evaluation of Alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Matos, H. A. S. (Ekstern), Gani, R. (Intern)
Publication date: 2008
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207763
Publication: Research - peer-review › Journal article – Annual report year: 2008

Development of sustainable chemical processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Gani, R. (Intern), Woodley, J. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 231449
Publication: Research › Poster – Annual report year: 2008

From property prediction to process and product design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 221009
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Increased Application Range of Property Models without New Experimental Data

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern), Khan, T. A. (Ekstern), Sen, S. (Ekstern), Bluck, D. (Ekstern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229280
Integrated design of solvent-based extractive separation processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Lek-utaiwan, P. (Ekstern), Gani, R. (Intern), Suphanit, B. (Ekstern), Mongkolsiri, N. (Ekstern)
Publication date: 2008

Model-based calculation of solid solubility for solvent selection – A review

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Modarresi, H. (Intern), Conte, E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern), Crafts, P. (Ekstern)
Pages: 5234-5242
Publication date: 2008
Main Research Area: Technical/natural sciences
Modeling and Analysis of Vacuum Membrane Distillation for the Recovery of Volatile Aroma Compounds from Black Currant Juice

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Pages: 442-455
Modelling and Simulation of Vegetable Oil Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Martinho, A. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern), Sarup, B. (Ekstern), Youngreen, W. (Ekstern)
Pages: 87-95
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Food and Bioproducts Processing
Volume: 82
ISSN (Print): 0960-3085
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.881 SNIP 1.178 CiteScore 2.59
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.182 SNIP 1.87 CiteScore 3.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.236 SNIP 2.098 CiteScore 3.24
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.932 SNIP 1.951 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.787 SNIP 1.703 CiteScore 2.36
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.643 SNIP 1.054 CiteScore 2.07
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.548 SNIP 0.745
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.358 SNIP 0.638
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.329 SNIP 0.576
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.264 SNIP 0.687
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.209 SNIP 0.486
Scopus rating (2005): SJR 0.261 SNIP 0.566
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.217 SNIP 0.459
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.342 SNIP 0.862
Models, modelling and Chemical Engineering – What Next?

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207766
Publication: Research - peer-review › Journal article – Annual report year: 2008

Off-line design of PAT systems for on-line applications

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 232290
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Off-line design of PAT systems for on-line applications

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Pages: 423-428
Publication date: 2008

Host publication information
Title of host publication: Computer Aided Chemical Engineering
Volume: 25
Main Research Area: Technical/natural sciences
Conference: 18th European Symposium on Computer Aided Process Engineering, Lyon, France, 01/06/2008 - 01/06/2008
Source: orbit
Source-ID: 220996
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008
Preface - Reklaitis 65th birthday special issue

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Venkatasubramanian, V. (Ekstern), Grossmann, I. (Ekstern), Gani, R. (Intern)
Pages: 631-632
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 32
Issue number: 4-5
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.293 SNIP 2.127
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.625 SNIP 1.959
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.304 SNIP 1.936
Scopus rating (2005): SJR 1.314 SNIP 1.953
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.125 SNIP 1.908
Web of Science (2004): Indexed yes
Properties in chemical process and product engineering: Needs, challenges and perspectives

General information
State: Submitted
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: O'Connell, J. (Ekstern), Gani, R. (Intern), Mathias, P. M. (Ekstern), Mawrer, G. (Ekstern), Olson, J. D. (Ekstern), Crafts, P. A. (Ekstern)
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Property Model Analysis for Use In Process-Product Development

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229161
Publication: Research › peer-review › Journal article – Annual report year: 2008
Solvents in Organic Synthesis: Replacement and Multi-step Reaction Systems

Solvents are widely used as reaction media in the chemical, fine chemical and pharmaceutical industries, but they present numerous environmental, health and safety (EHS) challenges that need to be managed and are subject to increasing regulatory scrutiny. The above issues, together with the principles of green chemistry, highlight the need to minimize and optimize the use of organic solvents as much as possible. One important step in optimizing organic solvent use is the identification of suitable ‘greener’ solvents that can help to minimize the environmental, health and safety concerns during design and commercial manufacture of chemical products. A method for selecting appropriate ‘greener’ solvents for the promotion of a class of organic reactions has been previously developed by Gani et al. This method employs estimates of thermodynamic properties to generate a knowledge base of reaction- and solvent-related properties that directly or indirectly influence a given reaction. In this work, the methodology has been extended through its application to several cases of increased process complexity involving multi-step reaction systems and solvent substitution for specific reaction steps in existing processing systems. The problems were formulated using the original methodology guidelines and incorporate knowledge of industrial practice in the currently available computer-aided tools for solvent design and property estimation. This presentation will describe the results obtained for a single reaction solvent screening problem, several solvent replacement problems and a multi-stage reaction system. In each example a list of solvent candidates is generated so they may be further investigated experimentally.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Gómez, P. A. (Ekstern), Folic, M. (Intern), Jiménez-González, C. (Ekstern), Constable, D. J. (Ekstern)
Pages: 2420-2444
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 32
Issue number: 10
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
Solvents In Organic Synthesis: Replacement and Multi-Step Reaction Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Gani, R. (Intern), Jimenez-Gonzalez, C. (Ekstern), Constable, D. (Ekstern), Shafique Bashir, M. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 205814
Publication: Research › Journal article – Annual report year: 2008

Special topic issue ECCE-6

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Kraslawski, A. (Ekstern), Morris, J. (Ekstern)
Pages: 661-661
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication Information
Journal: Chemical Engineering Research & Design
Volume: 86
Issue number: 7A
ISSN (Print): 0263-8762
Sustainability Analysis of Chemical Process Plants Using a Hybrid Heuristic and Indicator Model

**General Information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Halim, I. (Intern), Carvalho, A. (Ekstern), Srinivasan, R. (Ekstern), Gani, R. (Intern), Matos, H. A. S. (Ekstern)
Publication date: 2008

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229331
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Systematic Methodology for Continuous/ batch processes: analysis and generation of sustainable alternatives

**General Information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern)
Publication date: 2008

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 222458
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Systematic methodology for process analysis and generation of sustainable alternatives

**General Information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Gani, R. (Intern), Matos, H. A. (Ekstern)
Publication date: 2008

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 221019
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Systematic methodology for process analysis and generation of sustainable alternatives

**General Information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Gani, R. (Intern), Matos, H. A. (Ekstern)
Number of pages: 1,232
Publication date: 2008

**Host publication information**
Title of host publication: 18th European Symposium on Computer Aided Process Engineering
Publisher: Elsevier Science

Series: Computer - Aided Chemical Engineering
Volume: 25
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 18th European Symposium on Computer Aided Process Engineering , Lyon, France, 01/06/2008 - 01/06/2008
Systematic Modelling Framework in Chemical product-Process Design and development

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229274
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Systematic Selection and Design of Green Solvents for Organic Reacting Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Folic, M. (Intern), Gani, R. (Intern), Jiménez-González, C. (Ekstern), Constable, D. J. (Ekstern)
Pages: 376-383
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Chinese Journal of Chemical Engineering
Volume: 16
Issue number: 3
ISSN (Print): 1004-9541
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.37 SJR 0.404 SNIP 0.741
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.502 SNIP 1.111 CiteScore 1.61
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.56 SNIP 1.195 CiteScore 1.53
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.517 SNIP 1.197 CiteScore 1.4
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.545 SNIP 1.132 CiteScore 1.29
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.514 SNIP 1.07 CiteScore 1.36
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.493 SNIP 0.747
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.414 SNIP 0.775
BFI (2008): BFI-level 1
The Need and Use of Thermophysical Databases in Property Modeling and for Applications in Process-Product Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2008

Use of CAPE-OPEN standards in the interoperability between modelling tools (MoT) and process simulators (ProSim)

Computer-aided design, analysis and/or operation of chemical products and processes that manufacture them require a number of computational tools. As these tools may come from different sources and disciplines, an important issue is how they can be used simultaneously and efficiently for the design, analysis and/or simulation of a specific process-product? One alternative is to employ CAPE-OPEN standard interfaces for integration of the set of diverse computational tools that may be needed to solve the problem. The objective of this paper is to highlight, through examples, the integration of different computational tools according to problem specific work-flows/data-flows. The reliability of the integration of different tools is illustrated through two case studies. In case study 1, the tools Simulis® Thermodynamics (PME) and ICAS-MoT (PMC) are combined for the calculation of thermodynamic properties through the use of a standard middleware (DLL file). In case study 2, the interoperability between ProSimPlus simulator (PME) and ICAS-MoT (PMC) is highlighted for simulation of a new unit operation and combined with other unit operations that can be found in the host simulator. A ProSimPlus-ICAS-MoT-COFE interoperability is also carried out successfully to proof the interoperability of the different computational entities. Furthermore, the introduction of the multiscale modelling concept and its application through the CAPE-OPEN standards is highlighted.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 221011
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Use of property models in chemical process-product development – which, when & how?

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 221013
Publication: Research › Sound/Visual production (digital) – Annual report year: 2008

Use of Property Models in Chemical Process-Product Development – Which, When and How?

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Pages: 3-4
Publication date: 2008

Host publication information
Title of host publication: Proceedings of the 23rd European Symposium on Applied Thermodynamics
Editor: Jaubert, J.
Main Research Area: Technical/natural sciences
Conference: 23rd European Symposium on Applied Thermodynamics, Cannes, France, 29/05/2008 - 29/05/2008
Source: orbit
Source-ID: 250846
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008
Use of the Constrained FREE Energy Method for Multiphase Chemical REACTOR Simulation

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Koukkari, P. S. (Ekstern), Pajarre, R. (Ekstern), Gani, R. (Intern)
Publication date: 2008
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 229338
Publication: Research - peer-review › Poster – Annual report year: 2008


General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Pages: 141-146
Publication date: 2007
Host publication information
Title of host publication: Computer Aided Chemical Engineering
Volume: 24
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 201514
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007

A General Model and Its Analysis for Membrane Based Separation Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2007
Publication information
Publisher: Proceedings of ICAPP 2007
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208283
Publication: Research - peer-review › Report – Annual report year: 2007

A General Model and Its Analysis for Membrane Based Separation Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2007
Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207994
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007
A hierarchal approach based on reverse design algorithm for simultaneous design and analysis of product and processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Pages: 461-466
Publication date: 2007

Host publication information
Title of host publication: Computer-Aided Process Engineering
Volume: Volume 24
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 201515
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007

A method for prediction of UNIFAC group interaction parameters

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern), Rousseaux, P. (Ekstern), Le Bert, B. (Ekstern)
Pages: 1620-1632
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207991
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
A Methodology for Systematic Design and Selection of Green Solvents for Increased Yield in Organic Reactions

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Folic, M. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
A methodology for the design and selection of green solvents for organic reactions

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Folic, M. (Intern), Gani, R. (Intern), Jiménez-González, C. (Ekstern), Constable, D. J. (Ekstern)
Pages: 117-118
Publication date: 2007

Host publication information
Title of host publication: ECCE-6 Book of Abstracts
Volume: 1
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 206729
Publication: Research › Article in proceedings – Annual report year: 2007

A Model-Based Systems Approach for Innovation in Integrated Chemical Product-Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Morales Rodriguez, R. (Intern), Conte, E. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208007
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

An Experimental Verification of morphology of ibuprofen crystals from CAMD designed solvent

In our previous work [Karunanithi et al., 2006. A computer-aided molecular design framework for crystallization solvent design. Chemical Engineering Science 61, 1247-1260] we proposed a computer-aided molecular design (CAMD) framework to design solvents for crystallization processes. One of the important aspects of that work was the consideration of a qualitative property, namely crystal morphology, along with other physico-chemical properties (quantitative) of the solvents within the modeling framework. However, it is our view that consideration of any qualitative property, such as morphology of crystals formed from solvents, necessitates additional experimental verification steps. In this work we report the experimental verification of crystal morphology for the case study, solvent design for ibuprofen crystallization, presented in Karunanithi et al. [2006. A computer-aided molecular design framework for crystallization solvent design. Chemical Engineering Science 61, 1247-1260]. This we believe is an important step for the validation of the proposed solvent design model.
Application of Cape-Open Standards for the Interoperability between Computer-Aided Modelling Tools Mot and Process Simulators Prosimplus

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern), Vacher, A. (Ekstern), Castelain, P. (Ekstern), Dechelotte, S. (Ekstern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208032
Publication: Research › Article in proceedings – Annual report year: 2007

A Systematic Synthesis Framework for Extractive Distillation Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Kossack, S. (Ekstern), Kraemer, K. (Ekstern), Gani, R. (Intern), Marquardt, W. (Ekstern)
Pages: 557-558
Publication date: 2007

Host publication information
Title of host publication: ECCE-6 Book of Abstracts
Volume: 2
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 207003
Publication: Research › Article in proceedings – Annual report year: 2007
Chemical Product Design: Toward a Perspective through Case Studies

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Ng, K. M. (Ekstern), Gani, R. (Intern), Dam-Johansen, K. (Intern)
Number of pages: 501
Publication date: 2007

Publication information
Publisher: Elsevier
ISBN (Print): 978-0-444-52217-7
Original language: English
Series: Computer - Aided Chemical Engineering
Volume: 23
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Links:
Source: orbit
Source-ID: 193706
Publication: Research - peer-review › Book – Annual report year: 2007

Computer Aided Design, Analysis And Experimental Investigation Of Membrane Assisted Batch Reaction

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mitkowski, P. T. (Intern), Buchaly, C. (Ekstern), Kreis, P. (Ekstern), Jonsson, G. E. (Intern), Gani, R. (Intern), Górak, A. (Ekstern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208033
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Computer aided design and analysis of the hybrid processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mitkowski, P. T. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Pages: 769-781
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Inżynieria Chemiczna i Procesowa
Volume: 28
Original language: English
Source: orbit
Source-ID: 201509
Publication: Research - peer-review › Journal article – Annual report year: 2007
Computer aided design and analysis of the hybrid processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mitkowski, P. T. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207998
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Computer-Aided Framework for Pure Component Properties and Phase Equilibria Prediction for Organic Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Pages: 199-204
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 261
ISSN (Print): 0378-3812
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Computer aided modelling: Challenges and opportunities

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2007

Chemical processes are generally modeled through monoscale approaches, which, while not adequate, satisfy a useful role in product-process design. In this case, use of a multi-dimensional and multi-scale model-based approach has importance in product-process development. A computer-aided framework for model generation, analysis, solution and implementation is necessary for the development and application of the desired model-based approach for product-centric process design/analysis. This goal is achieved through the combination of a system for model development (ModDev), and a modelling tool (MoT) for model translation, analysis and solution. The integration of ModDev, MoT and ICAS or any other external software or process simulator (using COM-Objects) permits the generation of different models and/or process configurations for purposes of simulation, design and analysis. Consequently, it is possible to reduce time and human resources in the development and solution of models.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern)
Pages: 207-212
Computer-Aided Product Design – An Msc Course

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abildskov, J. (Intern), Gani, R. (Intern)
Pages: 691-692
Publication date: 2007

Host publication information
Title of host publication: ECCE-6 Book of Abstracts
Volume: 1
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 206878
Publication: Research › Article in proceedings – Annual report year: 2007

Design of Process Monitoring and Analysis Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208001
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Design of Process Monitoring and Analysis Systems, using a Model-based Computer Aided Framework

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Computer Aided Process Engineering Center
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Pages: 529-530
Publication date: 2007
**Design of Process Monitoring and Analysis Systems, using a Model-based Computer Aided Framework**

**General information**
State: Published  
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering  
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)  
Publication date: 2007

**Publication information**
Original language: English  
Main Research Area: Technical/natural sciences  
Source: orbit  
Source-ID: 208010  
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

**Design of Sustainable Processes: Systematic Generation & Evaluation of Alternatives**

**General information**
State: Published  
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering  
Authors: Carvalho, A. I. C. S. G. (Ekstern), Matos, H. A. S. (Ekstern), Gani, R. (Intern)  
Publication date: 2007

**Publication information**
Original language: English  
Main Research Area: Technical/natural sciences  
Source: orbit  
Source-ID: 208026  
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

**Development of Group Contribution Plus Property Models for Organic Systems**

**General information**
State: Published  
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering  
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)  
Pages: 105-106  
Publication date: 2007

**Host publication information**
Title of host publication: ECCE-6 Book of Abstracts  
Volume: 2  
Main Research Area: Technical/natural sciences  
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007  
Source: orbit  
Source-ID: 207000  
Publication: Research › Article in proceedings – Annual report year: 2007

**Development of Group Contribution Plus Property Models for Organic Systems**

**General information**
State: Published  
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Development of Polymer Property Prediction Models in Parallel Using Grid Technology

Examples of Multiscale Modelling in Chemical Product Design

Generating and Evaluating Entrainers for Extractive Distillation Processes in a Systematic Synthesis Framework

Group-contribution based method for surface tension estimation
Host publication information
Title of host publication: ECCE-6 Book of Abstracts
Volume: 2
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 206883
Publication: Research › Article in proceedings – Annual report year: 2007

Group-contribution based method for surface tension estimation

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Martinho, A. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208014
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Innovation in Integrated Chemical Product-Process Design – A Systems Approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208020
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Integrating Multilevel Modeling Aspects to Design the Membranes Using Reverse Design Algorithm

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Publisher: Proceedings of ICAPP 2007
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208288
Publication: Research - peer-review › Report – Annual report year: 2007

Integrating multilevel modeling aspects to predict gas permeability in polymers for design of membranes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Karayiannis, N. (Ekstern), Mavrantzas, V. (Ekstern)
Publication date: 2007
Integrating multilevel modeling aspects to predict gas permeability in polymers for design of membranes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Karayiannis, N. (Ekstern), Mavrantzas, V. (Ekstern)
Publication date: 2007

Integrating Multilevel Modelling Aspects to Design the Membranes Using Reverse Design Algorithm

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2007

Methodology for the design and analysis of reaction-separation systems with recycle. 1. The design perspective

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Ramirez Jimenez, E. (Intern), Gani, R. (Intern)
Pages: 8066-8083
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 46
Issue number: 24
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
Methodology for the design and analysis of reaction-separation systems with recycle. 2. Design and control algorithms

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Ramirez Jimenez, E. (Intern), Gani, R. (Intern)
Model-based Computer Aided Framework for Design of Process Monitoring and Analysis Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Computer Aided Process Engineering Center
Authors: Singh, R. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Publication date: 2007
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 201675
Publication: Research › Conference abstract for conference – Annual report year: 2007

Model-based hybrid reaction-separation process design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mitkowski, P. T. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Pages: 395-400
Publication date: 2007
Host publication information
Title of host publication: Computer Aided Chemical Engineering
Volume: 24
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 201516
Publication: Research › Article in proceedings – Annual report year: 2007

Modeling and simulation of vegetable oils process

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207990
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007
Modelling and simulation of vegetable oils process

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Martinho, A. (Ekstern), Matos, H. A. (Ekstern), Gani, R. (Intern), Sarup, B. (Ekstern), Youngreen, W. (Ekstern)
Publication date: 2007

Modelling of Chemical Systems to Predict Product Properties

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Abildskov, J. (Intern)
Publication date: 2007

Models, modeling and process systems engineering – what next?

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2007

Multiscale Modeling Aspects of Sustainable Product Engineering
Polymer property modeling using grid technology for design of structured products

Property prediction for a given polymer structure using group contribution models require that the structure can be fully represented by groups with well-defined contributions for that particular property. Frequently this cannot be accomplished. To overcome this limitation a group contribution(+) approach is developed here, for polymers. With this approach the missing groups are created and their contributions are predicted using zero- and first-order connectivity indices. To minimize the time spent on computational aspects of model development, grid technology is used in this work. Property prediction methods for linear polymers are presented for the amorphous and crystalline volumes, glass transition temperature, solubility parameter and refractive index. (c) 2007 Published by Elsevier B.V.
Polymer Property Modeling Using Grid Technology for Design of Structured Products

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207771
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Polymer Property Modelling for the Design of the Structured Products

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2007
Polymer property modelling using grid technology for design of structured products

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Pages: 1033-1034
Publication date: 2007

Host publication information
Title of host publication: ECCE-6 Book of Abstracts
Volume: 1
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 206880
Publication: Research › Article in proceedings – Annual report year: 2007

Process Systems Engineering and CAPE – what next?

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Grossmann, I. (Ekstern)
Pages: 1-6
Publication date: 2007

Host publication information
Title of host publication: Computer Aided Chemical Engineering
Volume: 24
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 201518
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Grossmann, I. (Ekstern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 221006
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Product Development – What to Make and How to Make

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Ng, K. M. (Ekstern), Gani, R. (Intern), Dam-Johansen, K. (Intern)
Pages: 473-489
Publication date: 2007

Host publication information
Title of host publication: Computer-Aided Chemical Engineering, 23
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193710
Publication: Research - peer-review › Book chapter – Annual report year: 2007

ProPred 4.0 User Guide

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Publisher: CAPEC-DTU
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 201534
Publication: Research - peer-review › Report – Annual report year: 2007

Selected papers from the 7th World Congress of Chemical Engineering, Glasgow, July 2005

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Bogle, D. (Ekstern), Gani, R. (Intern)
Pages: 875-875
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 31
Issue number: 8
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Simultaneous polymer property modeling using Grid technology for structured products
Simultaneous polymer property modeling using Grid technology for structured products

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Satyanarayana, K. C. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 201517
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007

Simultaneous product and processes design using reverse design algorithm

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2007

Host publication information
Title of host publication: ECCE-6 Book of Abstracts
Volume: 1
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 206882
Publication: Research › Article in proceedings – Annual report year: 2007

Simultaneous product and processes design using reverse design algorithm

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208004
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007
Use of CAPE-OPEN standards in the interoperability between modelling tools (MoT) and process simulators (ProSim)

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Gani, R. (Intern), Déchelotte, S. (Ekstern), Vacher, A. (Ekstern), Baudouin, O. (Ekstern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208013
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Development of a Computer Aided Modelling System for Bio and Chemical Process and Product Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Number of pages: 304
Publication date: May 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PEC06-17.pdf
Source: orbit
Source-ID: 188944
Publication: Research › Ph.D. thesis – Annual report year: 2006

Modelling, Design, Operability and Analysis of Reaction-Separation Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Jimenez, E. R. (Intern), Gani, R. (Intern)
Publication date: Mar 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PEC05-53.pdf
Source: orbit
Source-ID: 182598
Publication: Research › Ph.D. thesis – Annual report year: 2006

Prediction of solubility and diffusion properties of pesticides in polymers

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Suné, N. M. (Intern), Gani, R. (Intern)
A computer-aided molecular design framework for crystallization solvent design

One of the key decisions in designing solution crystallization processes is the selection of solvents. In this paper, we present a computer-aided molecular design (CAMD) framework for the design and selection of solvents and/or anti-solvents for solution crystallization. The CAMD problem is formulated as a mixed integer nonlinear programming (MINLP) model. Although, the model allows any combination of performance objectives and property constraints, in the case studies, potential recovery was considered as the performance objective. The latter, needs to be maximized, while other solvent, property requirements such as solubility, crystal morphology, flashpoint, toxicity, viscosity, normal boiling and melting point are posed as constraints. All the properties are estimated using group contribution methods. The MINLP model is then solved using a decomposition approach to obtain optimal solvent molecules. Solvent design and selection for two types of solution crystallization processes namely cooling crystallization and drowning out crystallization are presented. In the first case study, the design of single compound solvent for crystallization of ibuprofen, which is an important pharmaceutical compound, is addressed. One of the important issues namely, the effect of solvent on the shape of ibuprofen crystals is also considered in the MINLP model. The second case study is a mixture design problem where an optimal solvent/anti-solvent mixture is designed for crystallization of ibuprofen by the drowning out technique. For both case studies the performance of the solvents are verified qualitatively through SLE diagrams. (c) 2005 Elsevier Ltd. All rights reserved.
A Modern Approach to Solvent Selection

General information
A Simple New Concept for Chemical Process Flowsheet Design and Analysis

CAPEC Research Report 2006

Computer aided design of hybrid processes consisting of reactor and membrane-based separation unit
Computer Aided Methodology for Simultaneous Synthesis, Design & Analysis of Chemical Products-Processes

A new combined methodology for computer aided molecular design and process flowsheet design is presented. The methodology is based on the group contribution approach for prediction of molecular properties and design of molecules. Using the same principles, process groups have been developed together with their corresponding flowsheet property models. To represent the process flowsheets in the same way as molecules, a unique but simple notation system has been developed. The methodology has been converted into a prototype software, which has been tested with several case studies covering a wide range of problems. In this paper, only the computer aided flowsheet design related features are presented.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: d'Anterroches, L. (Intern), Gani, R. (Intern)
Pages: 853-858
Publication date: 2006

Host publication information
Title of host publication: Proceedings of the 16th European Symposium on Computer Aided Process Engineering and the 9th Symposium on Process Systems Engineering
Publisher: Elsevier Science
Series: Computer - Aided Chemical Engineering
Volume: 21
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Molecular design, flowsheet design, product, process, group-contribution
DOIs: 10.1016/S1570-7946(06)80152-5
Source: orbit
Source-ID: 188934
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006

An integrated approach that is particularly suitable for solving problems related to product-process design from the fine chemicals, agrochemicals, food and pharmaceutical industries is presented together with the corresponding methods and tools, which forms the basis for an integrated computer aided system. The methods and tools are linked through the problems they are able to solve and the associated data-flow. The integrated computer aided system has been used to solve a number of industrial problems and summarized results from a selection, involving separation and purification issues, are presented.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Authors: Afonso, M. B. (Ekstern), Soni, V. (Intern), Mitkowski, P. T. (Intern), d'Anterroches, L. (Intern), Gani, R. (Intern), Matos, H. (Ekstern)
Pages: 805-810
Publication date: 2006

Host publication information
Title of host publication: Proceedings of the 16th European Symposium on Computer Aided Process Engineering and the 9th Symposium on Process Systems Engineering
Publisher: Elsevier Science

Series: Computer - Aided Chemical Engineering
Volume: 21
ISSN: 1570-7946
Main Research Area: Technical/natural sciences

Fine chemicals, agrochemicals, food, pharmaceutical products, separation, purification, methods and tools

DOIs: 10.1016/S1570-7946(06)80144-6

Source: orbit
Source-ID: 190522
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006


The advances in computer science and computational algorithms for process modelling, process simulation, numerical methods and design/synthesis algorithms, makes it advantageous and helpful to employ computer-aided modelling systems and tools for integrated process analysis. This is illustrated through the study of a copolymerization process, where operational problems due to their complex nonlinear behaviour are usually encountered, indicating thereby, the need for the development of an appropriate process model that can describe the dynamic behaviour over the complete range of conversion. This will allow analysis of the process behaviour, contribute to a better understanding of the polymerization process, help to avoid unsafe conditions of operation, and to develop operational and optimizing control strategies. In this work, through a computer-aided modeling system ICAS-MoT, two first-principles models have been investigated with respect to design and operational issues for solution copolymerization reactors in general, and for the methyl methacrylate/vinyl acetate system in particular. The Model 1 is taken from literature and is commonly used for low conversion region, while the Model 2 has been derived in this work and covers the complete range of conversion. The performances of the two models are compared with respect to the steady state and dynamic behaviour of the...
polymerization process. The model analyses highlight the influence of the reaction mechanism, the transport phenomena, the process design and conditions of operation on the polymer grade and the production rate.

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Lopez-Arenas, M. T. (Intern), Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Pages: 911-931
Publication date: 2006
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Chemical Engineering Research & Design
Volume: 84
Issue number: A10
ISSN (Print): 0263-8762
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.855 SNIP 1.449 CiteScore 2.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.957 SNIP 1.668 CiteScore 2.56
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.912 SNIP 1.335 CiteScore 2.12
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.87 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.742 SNIP 1.029
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.645 SNIP 0.718
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.572 SNIP 0.787
Scopus rating (2006): SJR 0.629 SNIP 0.823
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.752 SNIP 1.02
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.609 SNIP 0.951
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.722 SNIP 0.704
An important stage in the design process for many chemical products is its manufacture where, for a class of chemical products that may be thermally unstable (such as, drugs, insecticides, flavours /fragrances, and so on), the purification step plays a major role. Short-path evaporation is a safe method, suitable for separation and purification of thermally unstable materials whose design and analysis can be efficiently performed through reliable model-based techniques. This paper presents a generalized model for short-path evaporation and highlights its development, implementation and solution through a computer-aided modelling framework, which allows the use of systematic simulation strategies for various types of design/analysis problems. The main features of the model and the modelling framework are highlighted through two case studies: (a) the purification of a reaction mixture containing glycerol, mono-, di- and triglycerides, and (b) the recovery of a pharmaceutical product from a six-component mixture. Validation of the short-path evaporation model is highlighted through the comparison of experimental data from an industrial pilot plant with the simulated results from the model. Also, results from model-based sensitivity analysis and design problem solution are highlighted for two case studies.
Computer aided modul-based design and analysis of hybrid membrane-reaction-separation processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Jonsson, G. E. (Intern), Mitkowski, P. T. (Intern), Soni, V. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190969
Publication: Research - peer-review → Journal article – Annual report year: 2006

Computer Aided Polymer Design Using Group Contribution Techniques

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Hostrup, M. (Ekstern), Harper, P. M. (Ekstern), Moen, Ø. (Ekstern), Suñé, N. M. (Ekstern), Soni, V. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2006
Computer-Aided Product Design – an M.Sc. Course

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193670
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Computer-aided Pure Component Property Prediction for Isomers

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190980
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Computer-aided Pure Components Property Prediction for Isomers

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190977
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Design of Sustainable Chemical Processes: Systematic Retrofit Analysis and Generation & evaluation of alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Matos, H. (Ekstern), Gani, R. (Intern)
Publication date: 2006
Design of sustainable processes: Systematic generation & evaluation of alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Authors: Carvalho, A. (Ekstern), Gani, R. (Intern), Matos, H. (Ekstern)
Pages: 817-822
Publication date: 2006

Host publication information
Title of host publication: Computer-Aided Chemical Engineering
Volume: 21A
Source: orbit
Source-ID: 188932
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006

Design of Sustainable Processes: Systematic Generation & Evaluation of Alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. (Ekstern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 197495
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Development of Group ContributionPlus Models for Properties of Organic Chemical Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Pages: 176-177
Publication date: 2006

Host publication information
Title of host publication: Dansk Kemiingeniørkonference – DK2-2006
Publisher: DK2
Main Research Area: Technical/natural sciences
Conference: 2. Dansk Kemiingeniørkonference, Kgs.Lyngby, Denmark, 31/05/2006 - 31/05/2006
Source: orbit
Source-ID: 191276
Publication: Research › Article in proceedings – Annual report year: 2006

Enzyme recovery by crossflow electro-ultrafiltration

General information
Generic hybrid models of solvent-based reactive systems combined with membrane separation

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Membrane Technology group
Authors: Mitkowski, P. T. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190978
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006
Integrated Chemical Product-Process Design: CAPE Perspectives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Pages: 647-666
Publication date: 2006

Host publication information
Title of host publication: Computer Aided Process-Product Engineering – CAPE
Volume: Section 4
Place of publication: Germany
Publisher: Wiley Interscience
Editors: Heyen, G., Puigjaner, L.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 181206
Publication: Research - peer-review › Book chapter – Annual report year: 2006

Integrated Computer-Aided Methods and Tools as Educational Modules

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Abildskov, J. (Intern)
Pages: 773-798
Publication date: 2006

Host publication information
Title of host publication: Computer Aided Process-Product Engineering - CAPE
Volume: Section 5
Place of publication: Germany
Publisher: Wiley Interscience
Editors: Heyen, G., Puigjaner, L.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 181207
Publication: Research - peer-review › Book chapter – Annual report year: 2006

Interoperability between Modelling Tools (Mot) and Process Simulators (Prosim) through Cape-Open Standards

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morales Rodriguez, R. (Intern), Sales-Cruz, A. M. (Intern), Gani, R. (Intern), Déchelotte, S. (Ekstern), Vacher, A. (Ekstern), Baudouin, O. (Ekstern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193674
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Mathematical and Numerical Analysis of Classes of Property Models

General information
Publication information
Journal: Fluid Phase Equilibria
Volume: 250
ISSN (Print): 0378-3812
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Model and Analysis of Vacuum Membrane Distillation for the Recovery of Volatile Aroma Compounds from Black Currant Juice

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Membrane Technology group
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 188946
Publication: Research › Journal article – Annual report year: 2006

Model Based Design of Structured Polymers Using the Reverse Design Approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Pages: 166-167
Publication date: 2006

Host publication information
Title of host publication: Dansk Kemiingeniørkonference – DK2-2006
Place of publication: Lyngby
Publisher: DK2
Main Research Area: Technical/natural sciences
Conference: 2. Dansk Kemiingeniørkonference, Kgs.Lyngby, Denmark, 31/05/2006 - 31/05/2006
Source: orbit
Source-ID: 191274
Publication: Research › Article in proceedings – Annual report year: 2006

Model-based reverse design of structured polymers

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Membrane Technology group
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Karayannis, N. (Ekstern), Mavrantzaz, V. (Ekstern)
Publication date: 2006
Event: Poster session presented at 3rd International Conference on Foundations of Molecular Modeling and Simulation, Blaine, WA, United States.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190972
Publication: Research - peer-review › Poster – Annual report year: 2006
Model discrimination and parameter estimation through sensitivity analysis

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sales Cruz, A. M. (Intern), Gani, R. (Intern)
Pages: 625-631
Publication date: 2006

Host publication information
Title of host publication: Computer-Aided Chemical Engineering
Volume: 21A
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 188929
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006

Multiscale property modeling for design of polymer based products

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Karayiannis, N. C. (Ekstern), Mavrantzas, V. (Ekstern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 191063
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

New Approach to Chemical Product-Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 188941
Publication: Research - peer-review › Paper – Annual report year: 2006
Prediction of Missing UNIFAC Group-interaction Parameters through Connectivity Indices

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gonzalez Villalba, H. E. (Intern), Le Bert, B. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190976
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Prediction Solubilities of Medium-Sized Complex Chemicals in Liquid Solvents. Retrieval, Reduction and Application

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abildskov, J. (Intern), Janot, J. (Ekstern), Christensen, M. (Ekstern), Gani, R. (Intern), Sass, R. (Ekstern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 191000
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006
Simultaneous Model-based Process and Product Design Using Reverse Design Approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Mitkowski, P. T. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193673
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Static/dynamic analysis and controllability issues in reactive distillation columns

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: López-Arenas, T. (Ekstern), Perez-Cisneros, E. S. (Ekstern), Gani, R. (Intern)
Pages: 1323-1328
Publication date: 2006

Host publication information
Title of host publication: Computer-Aided Chemical Engineering
Volume: 21B
Main Research Area: Technical/natural sciences
Source-ID: 188930
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006

Static/dynamic analysis and controllability issues in reactive distillation columns

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Lopez-Arenas, M. T. (Intern), Pérez-Cisneros, E. S. (Ekstern), Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 191064
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Structural design of polymers for membrane based separation processes using reverse simulation approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Karayiannis, N. (Ekstern), Mavrantzas, V. (Ekstern)
Pages: 689-699
Publication date: 2006

Host publication information
Title of host publication: Computer-Aided Chemical Engineering
Volume: 21A
Main Research Area: Technical/natural sciences
Structural design of polymers for membrane based separation processes using reverse simulation approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Membrane Technology group
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Karayiannis, N. (Ekstern), Mavrantzas, V. (Ekstern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 188931
Publication: Research › Article in proceedings – Annual report year: 2006

Systematic computer aided approach to product-process analysis and design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 190975
Publication: Research › Sound/Visual production (digital) – Annual report year: 2006

Systematic Computer-Aided Techniques for Use in Formulated Chemical Product Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Gani, R. (Intern)
Publication date: 2006
Event: Paper presented at 4th World Congress on Emulsions, Lyon, France, 3-6 October, .
Main Research Area: Technical/natural sciences
Source: orbit
Systematic model-based synthesis design and analysis of hybrid processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Membrane Technology group
Authors: Soni, V. (Intern), Mitkowski, P. T. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2006

Thermal pretreatment of the solid fraction of manure: Impact on the biogas reactor performance and microbial community

Application of thermal treatment at 100-140 degrees C as a pretreatment method prior to anaerobic digestion of a mixture of cattle and swine manure was investigated. In a batch test, biogasification of manure with thermally pretreated solid fraction proceeded faster and resulted in the increase of methane yield. The performances of two thermophilic continuously stirred tank reactors (CSTR) treating manure with solid fraction pretreated for 40 minutes at 140 degrees C and non-treated manure were compared. The digester fed with the thermally pretreated manure had a higher methane productivity and an improved removal of the volatile solids (VS). The properties of microbial communities of both reactors were analysed. The specific methanogenic activity (SMA) test showed that both biomasses had significant activity towards hydrogen and formate, while the activity with the VFA - acetate, propionate and butyrate - was low. The kinetic parameters of the VFA conversion revealed a reduced affinity of the microbial community from the CSTR fed with thermally pre-treated manure for acetate, propionate and butyrate. The bacterial and archaeal populations identified by 16S rRNA genes were found to be identical in both systems. However, a change in the abundance of the species present was detected.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Bioscience and Technology, Department of Systems Biology
Authors: Mladenovska, Z. (Ekstern), Hartmann, H. (Ekstern), Kvist, T. (Ekstern), Sales-Cruz, A. M. (Intern), Gani, R. (Intern), Ahring, B. K. (Intern)
Pages: 59-67
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Water Science and Technology
Volume: 53
Issue number: 8
ISSN (Print): 0273-1223
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.3 SJR 0.394 SNIP 0.621
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.466 SNIP 0.599 CiteScore 1.19
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.587 SNIP 0.685 CiteScore 1.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Towards More Sustainable Pharmaceutical Syntheses: Finding Solvent Replacements

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
A Computer Aided Framework for Efficient Formulation Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Muro Sunè, N. (Intern), Munir, A. (Ekstern), Bell, G. (Ekstern), Shirley, I. (Ekstern), Siemanond, K. (Ekstern)
Publication date: 2005

Host publication information
Title of host publication: 7th World Congress of Chemical Engineering : WCCE 7
Volume: CD-ROM
Main Research Area: Technical/natural sciences
Conference: 7th World Congress of Chemical Engineering, Glasgow, United Kingdom, 10/07/2005 - 10/07/2005
Source: orbit
Source-ID: 181201
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

A framework for product analysis: Modelling and design of release and uptake of pesticides
This paper presents a framework for chemical product (pesticide) design and analysis. The framework consists of a set of computer-aided methods and tools that have been integrated to tackle the needs with respect to solution of chemical product design problems related to pesticide formulations. Two of the mathematical models (controlled release and pesticide uptake) that provide the principal calculation options are highlighted together with selected results from case studies.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Muro Sunè, N. (Intern), Munir, A. (Ekstern), Gani, R. (Intern), Bell, G. (Ekstern), Shirley, I. (Ekstern)
Pages: 733-738
Publication date: 2005

Host publication information
Title of host publication: European Symposium on Computer-Aided Process Engineering-15
Volume: 20a-20b
Publisher: Elsevier Science B.V.
Editors: Puigjaner, L., Espuma, A.
ISBN (Print): 0-444-51987-4

Series: Computer - Aided Chemical Engineering
Volume: 20a-20b
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 15th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 29/05/2005 - 29/05/2005
Source: orbit
Source-ID: 182375
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

A framework for product analysis: Modelling and design of release and uptake of pesticides

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Muro Sunè, N. (Intern), Munir, A. (Ekstern), Gani, R. (Intern), Bell, G. (Ekstern), Shirley, I. (Ekstern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
A new decomposition-based computer-aided molecular/mixture design methodology for the design of optimal solvents and solvent mixtures

This paper presents a novel computer-aided molecular/mixture design (CAMD) methodology for the design of optimal solvents and solvent mixtures. The molecular/mixture design problem is formulated as a mixed integer nonlinear programming (MINLP) model in which a performance objective is to be optimized subject to structural, property, and process constraints. The general molecular/mixture design problem is divided into two parts. For optimal single-compound design, the first part is solved. For mixture design, the single-compound design is first carried out to identify candidates and then the second part is solved to determine the optimal mixture. The decomposition of the CAMD MINLP model into relatively easy to solve subproblems is essentially a partitioning of the constraints from the original set. This approach is illustrated through two case studies. The first case study involves the design of an optimal extractant for the separation of acetic acid from water by liquid-liquid extraction. The results suggest that the new extractant would be able to perform better than the extractant being widely used for this separation. The second case study is an industrial problem involving the optimal formulation for a pharmaceutical compound. The designed formulation is able to improve the water solubility of the compound by more many fold.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, University of Connecticut
Authors: Karunanithi, A. (Ekstern), Achenie, L. (Ekstern), Gani, R. (Intern)
Pages: 4785-4797
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 44
Issue number: 13
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
A New Retrofit Design Methodology for Identification, Developing and Evaluating Retrofit Projects for Cost-Efficiency Improvements in Continuous Chemical Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Uerdingen, E. (Ekstern), Fischer, U. (Ekstern), Gani, R. (Intern), Hungerbühler, K. (Ekstern)
Pages: 1842-1853
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 49
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Automatic Creation of Missing Groups through Connectivity Index for Pure Component Property Prediction

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Harper, P. M. (Ekstern), Hostrup, M. (Ekstern)
Pages: 7262-7269
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
CAPEC Research Report 2005

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 181205
Publication: Research - peer-review › Journal article – Annual report year: 2005

Conceptual Design and Synthesis of Batch Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Papaoikonomou, E. (Intern)
Pages: 43-82
Publication date: 2005

Host publication information
Title of host publication: Batch Processes
Place of publication: Boca Raton, USA
Publisher: CRC Publications
Editors: Linniger, A., Kororessi, E.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 181948
Publication: Research › Report – Annual report year: 2005

Crystal morphology considerations in processing of pharmaceutical drugs: A computer aided molecular design (CAMD) approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Karunanithi, A. T. (Ekstern), Achenie, L. E. (Ekstern), Gani, R. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 181211
Publication: Research › Book chapter – Annual report year: 2006

Design and Control Structure Integration from a Model-Based Methodology for Reaction-Separation with Recycle Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Jimenez, E. R. (Intern), Gani, R. (Intern)
Pages: 1519-1524
Publication date: 2005
Design and Control Structure Integration from a Model-Based Methodology for Reaction-Separation with Recycle Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Jimenez, E. R. (Intern), Gani, R. (Intern)
Publication date: 2005

Publication Information
Original language: English
Main Research Area: Technical/natural sciences
Source-ID: 183900
Publication: Research › Sound/Visual production (digital) – Annual report year: 2005

Design and Operation of Copolymerisation Reactors through Modelling and Nonlinear Analysis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Lopez-Arenas, M. T. (Intern), Sales Cruz, A. M. (Intern), Gani, R. (Intern)
Pages: 439-444
Publication date: 2005

Host publication information
Title of host publication: Computer Aided Chemical Engineering
Volume: Vol. 20
Publisher: Elsevier Science
Main Research Area: Technical/natural sciences
Conference: 15th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 29/05/2005 - 29/05/2005
Source-ID: 155055
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

Design of Molecules, Mixtures and Processes through a Novel Group Contribution Method

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: d'Anterroches, L. (Intern), Gani, R. (Intern), Harper, P. M. (Ekstern), Hostrup, M. (Ekstern)
Publication date: 2005

Host publication information
Title of host publication: 7th World Congress of Chemical Engineering – WCCE 7
Volume: CD-ROM
Main Research Area: Technical/natural sciences
Conference: 7th World Congress of Chemical Engineering, Glasgow, United Kingdom, 10/07/2005 - 10/07/2005
Source-ID: 182380
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005
Design of sustainable chemical processes: Systematic retrofit analysis and generation & evaluation of alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Carvalho, A. I. (Ekstern), Gani, R. (Intern), Matos, H. A. (Ekstern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 184822
Publication: Research › Sound/Visual production (digital) – Annual report year: 2005

Design of Sustainable Processes: Systematic Generation & Evaluation of Alternatives

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Jørgensen, S. B. (Intern), Jensen, N. (Intern)
Publication date: 2005

Host publication information
Title of host publication: 7th World Congress of Chemical Engineering
Volume: CD-ROM
Main Research Area: Technical/natural sciences
Conference: 7th World Congress of Chemical Engineering, Glasgow, United Kingdom, 10/07/2005 - 10/07/2005
Source: orbit
Source-ID: 181202
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

Dynamic analysis and controllability issues in reactive distillation columns

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Lopez-Arenas, M. T. (Intern), Perez-Cisneros, E. S. (Ekstern), Gani, R. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 184820
Publication: Research › Sound/Visual production (digital) – Annual report year: 2005

Enhancement of the organic matter removal during a two-step process for the anaerobic digestion of primary and secondary sludge: kinetic characterization and modelling

General information
State: Published
Organisations: Department of Systems Biology, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Bioscience and Technology
Authors: Skiadas, I. V. (Intern), Sales-Cruz, A. M. (Intern), Gavala, H. N. (Intern), Gani, R. (Intern), Ahring, B. K. (Intern)
Pages: 383-390
Publication date: 2005

Host publication information
Title of host publication: Proceedings of the 4th International Symposium on Anaerobic Digestion of Solid Waste
Volume: Volume 1 - Oral presentations
Publisher: Publisher unknown
Main Research Area: Technical/natural sciences
Conference: 4th International Symposium on Anaerobic Digestion of Solid Waste, Copenhagen, Denmark, 31/08/2005 - 31/08/2005
Estimation of enthalpy of vaporization and of entropy of vaporization for pure organic compounds at 298.15 K and at normal boiling temperature by a group contribution method

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kolská, Z. (Ekstern), Ruzická, V. (Ekstern), Gani, R. (Intern)
Pages: 8436-8454
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 44
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Generation and Evaluation of Sustainable Process Alternatives for Improved Safety using an Integrated Computer Aided System

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Jensen, N. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 183852
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

Host publication information
Title of host publication: 2nd Annual International Conference on Integration of Environmental Problems with the Theory of Sustainable Developments into the Management System in Enterprises
Main Research Area: Technical/natural sciences
Conference: 2nd Annual International Conference on Integration of Environmental Problems with the Theory of Sustainable Developments into the Management System in Enterprises, Bialystok, Poland, 17/01/2005 - 17/01/2005
Source: orbit
Source-ID: 154983
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

Generation and evaluation of sustainable process (retrofit) alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2005
In a group contribution method for pure component property prediction, a molecule is described as a set of groups linked together to form a molecular structure. In the same way, for flowsheet "property" prediction, a flowsheet can be described as a set of process-groups linked together to represent the flowsheet structure. Just as a functional group is a collection of atoms, a process-group is a collection of operations forming an "unit" operation or a set of "unit" operations. The link between the process-groups are the streams similar to the bonds that are attachments to atoms/groups. Each process-group provides a contribution to the "property" of the flowsheet, which can be performance in terms of energy consumption, thereby allowing a flowsheet "property" to be calculated, once it is described by the groups. Another feature of this approach is that the process-group attachments provide automatically the flowsheet stream properties, which serves as very good initial estimates for convergence of mass/energy balance calculations. (c) 2004 Elsevier B.V. All rights reserved.
Hybrid process design-analysis in pharmaceutical and biochemical industry

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Mitkowski, P. T. (Ekstern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 132447
Publication: Research › Conference article – Annual report year: 2005

Integrated Chemical Product-Process Design: CAPE Perspectives

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Pages: 21-30
Publication date: 2005
Method for Selection of Solvents for Promotion of Organic Reactions

A method to select appropriate green solvents for the promotion of a class of organic reactions has been developed. The method combines knowledge from industrial practice and physical insights with computer-aided property estimation tools for selection/design of solvents. In particular, it employs estimates of thermodynamic properties to generate a knowledge base of reaction, solvent and environment related properties that directly or indirectly influence the rate and/or conversion of a given reaction. Solvents are selected using a rules-based procedure where the estimated reaction-solvent properties and the solvent-environmental properties guide the decision making process. The current method is applicable only to organic reactions occurring in the liquid phase. Another gas or solid phase, which may or may not be at equilibrium with the reacting liquid phase, may also be present. The objective of this method is to produce, for a given reaction, a short list of chemicals that could be considered as potential solvents, to evaluate their performance in the reacting system, and, based on this, to rank them according to a scoring system. Several examples of application are given to illustrate the main features and steps of the method. (c) 2005 Elsevier Ltd. All rights reserved.
Model and Analysis of Vacuum Membrane Distillation for the Recovery of Volatile Aroma Compounds from Black Currant Juice

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern)
Publication date: 2005
Main Research Area: Technical/natural sciences
Model-based computer-aided design for controlled release of pesticides

In the field of controlled release technology for pesticides or active ingredients (AI), models that can predict its delivery during application are important for purposes of design and marketing of the pesticide product. Appropriate models for the controlled release of pesticides, if available, can be used to study and analyze some of the important issues related to the design/application of the pesticide. This paper highlights the needs for predictive models and proposes the use of a computer aided modelling framework through which a collection of reliable and predictive constitutive (property) models can be combined with various types of release models. Use of a group-contribution based property model for one of the constitutive variables (AI solubility in polymers) and a free-volume theory based model for another (diffusion coefficient), has been proposed and the corresponding extended models have been developed and implemented into a computer-aided system. The total model consisting of the property models embedded into the release models are then employed to study the release of different combinations of AIs and polymer-based microcapsules.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Muro Sunè, N. (Intern), Gani, R. (Intern), Bell, G. (Ekstern), Shirley, I. (Ekstern)
Pages: 28-41
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Computers & Chemical Engineering
Volume: 30
Issue number: 1
ISSN (Print): 0098-1354
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.161 SNIP 1.92 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.185 SNIP 1.736 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.176 SNIP 1.796
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.154 SNIP 2.166
Modelling of Acute Exposure Guideline Levels using Group Contribution Methods

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Jensen, N. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 198329
Publication: Research - peer-review › Journal article – Annual report year: 2005

Modelling of Acute Exposure Guideline Levels using Group Contribution Methods

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Jensen, N. (Intern), Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2005

Host publication information
Title of host publication: 7th World Congress of Chemical Engineering : WCCE7
Volume: CD-ROM
Main Research Area: Technical/natural sciences
Conference: 7th World Congress of Chemical Engineering, Glasgow, United Kingdom, 10/07/2005 - 10/07/2005
Source: orbit
Source-ID: 154980
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005
Predictive property models for use in design of controlled release of pesticides

A model capable of predicting the release of an Active Ingredient (AI) from a specific device would be very useful in the field of pesticide controlled release technology for design purposes. For the release of an AI from a microcapsule a mathematical model is briefly presented here, as an introduction to the principal objective of this work, which is the prediction of the model parameters (diffusion and partition coefficients). In particular, this paper focuses on the estimation of the partition coefficient of the AI in the polymer through activity coefficients, that are estimated with a group-contribution model for polymers (GC-Flory EoS). Therefore, this model (GC-Flory EoS) is extended in order to suit the needs of the complex pesticide molecules. The results of the extension of the GC-Flory EoS model, together with a case study dealing with the release of a pesticide from a microcapsule as well as the estimation of model parameters are presented. (c) 2004 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Suné, N. M. (Intern), Gani, R. (Intern), Bell, G. (Ekstern), Shirley, I. (Ekstern)
Pages: 127-133
Publication date: 2005
Conference: 10th International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, UT, United States, 16/05/2004 - 16/05/2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 228-229
Issue number: SI
ISSN (Print): 0378-3812
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
Recent Developments in the Modelling of Thermodynamic Properties for Computer-Aided Process and Product Engineering Applications

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Abildskov, J. (Intern), Gani, R. (Intern)
Pages: 30-32
Publication date: 2005

Host publication information
Title of host publication: Proceedings of 21st European Symposium on Applied Thermodynamics: (ESAT 2005)
Main Research Area: Technical/natural sciences
Conference: 21st European Symposium on Applied Thermodynamics, Jurata, Poland, 01/06/2005 - 01/06/2005
Source: orbit
Source-ID: 181949
Publication: Research › Article in proceedings – Annual report year: 2005

Recent Developments in the Modelling of Thermodynamic Properties for Computer-Aided Process and Product Engineering Applications

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 184810
Short-Path Evaporation for Chemical Product Modelling, Analysis and Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sales Cruz, A. M. (Intern), Gani, R. (Intern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 184802
Publication: Research › Sound/Visual production (digital) – Annual report year: 2005

Short-Path Evaporation for Chemical Product Modelling, Analysis and Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Sales Cruz, A. M. (Intern), Gani, R. (Intern)
Pages: 841-846
Publication date: 2005

Host publication information
Title of host publication: Computer Aided Chemical Engineering
Volume: Vol. 20
Publisher: Elsevier Science B.V.
Main Research Area: Technical/natural sciences
Conference: 15th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 29/05/2005 - 29/05/2005
Source: orbit
Source-ID: 155052
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

Structural Design of Polymers for Membrane Based Separation Using Reverse Simulation Approach

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Soni, V. (Intern), Abildskov, J. (Intern), Jonsson, G. E. (Intern), Gani, R. (Intern), Karayiannis, N. C. (Ekstern), Mavrantzas, V. (Ekstern)
Publication date: 2005

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 183086
Publication: Research › Sound/Visual production (digital) – Annual report year: 2005

The Reverse Approach for Synthesis and Design of Chemical Products & Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: d’Anterroches, L. (Intern), Gani, R. (Intern)
Publication date: 2005

Host publication information
Title of host publication: 7th World Congress of Chemical Engineering : WCCE 7
Thermal treatment of the solid fraction of manure: Impact on the biogas reactor performance and microbial community

**General information**

State: Published
Organisations: Bioscience and Technology, Department of Systems Biology, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Mladenovska, Z. (Intern), Uellendahl (Hartmann), H. (Intern), Kvist, T. (Intern), Sales Cruz, A. M. (Intern), Gani, R. (Intern), Ahring, B. K. (Intern)
Pages: 218-225
Publication date: 2005

**Host publication information**

Title of host publication: 4th International Symposium Anaerobic Digestion of Solid Waste
Volume: 1
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 182382
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

A Computer-Aided Modelling Framework Applied to a Polymerisation Process

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Publication date: 2004
Event: Poster session presented at Dansk Kemiingeniørkonference, Lyngby, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 154179
Publication: Research › Poster – Annual report year: 2004

Actuator selection based upon model insights for an energy integrated distillation column

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2004

**Publication information**

Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135915
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Actuator Selection Based Upon Model Insights for an Energy Integrated Distillation Column

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Pages: 135-140
Publication date: 2004
A methodology for the analysis and design of reaction-separation recycle systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ramirez Jimenez, E. (Intern), Gani, R. (Intern)
Publication date: 2004

A Methodology for the Analysis and Design of Reaction-Separation-Recycle Systems

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Ramirez Jimenez, E. (Intern)
Pages: 315-318
Publication date: 2004

A Methodology for the Design of Reaction-Separation Systems with Recycle

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ramirez Jimenez, E. (Intern), Gani, R. (Intern)
Publication date: 2004
Event: Poster session presented at Dansk Kemilærenkonference, Lyngby, Denmark.


General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Sales-Cruz, A. M. (Intern)
Pages: 581-585
Publication date: 2004
A modelling framework for chemical process design through a computer aided system

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135925
Publication: Research - peer-review › Article in proceedings – Annual report year: 2004

Analysis of optimal operation of an energy integrated distillation plant

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Hansen, C. A. (Ekstern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135884
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

An Integrated Computer Aided System for Generation and Evaluation of Sustainable Process Alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Jensen, N. (Intern), Coll, N. (Ekstern), Gani, R. (Intern)
Publication date: 2004

Publication information
Host publication information
Title of host publication: Technological Choices for Sustainability
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 154490
Publication: Research - peer-review › Book chapter – Annual report year: 2004

A novel framework for simultaneous separation process and product design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Eden, M. R. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), El-Halwagi, M. M. (Ekstern)
Pages: 595-608
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Application of Property Models in Chemical Product Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Aspects of modelling and model identification for bioprocesses through a computer-aided modelling system

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135887
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

A systematic approach for the design and analysis of reaction-separation systems with recycle

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Ramirez Jimenez, E. (Intern), Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135889
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

A Systematic Approach for the Design and Analysis of Reaction-Separation Systems with Recycle
This paper presents a methodology for a systematic model-based analysis and the results obtained from it for an integrated design and analysis of reaction-separation systems with recycle. The methodology (systematic approach) consists of three stages where stage 1 identifies the limiting values of the design/operation variables; stage 2 identifies the
goal/target values of a related set of design/operation variable's and stage 3 verifies/validates the result of stages 1 and 2. The methodology decomposes the problem in such way that every stage generates information (data) and resolves a subset of design and operational issues. This information generation is cumulative so that at the last stage all-important (and relevant) data of the process becomes known while all-important design and operation issues become resolved. Two reaction-separation systems have been chosen as preliminary case studies to illustrate the methodology. The first example considers a second-order reaction while the second example comprises a consecutive first-order reaction system.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Jimenez, E. R. (Ekstern)
Pages: 469-474
Publication date: 2004

Host publication information
Title of host publication: Computer Aided Chemical Engineering - 14
Publisher: Elsevier Science
ISBN (Print): 0-444-51694-8
Series: Computer - Aided Chemical Engineering
Volume: 18
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 14th European Symposium on Computer Aided Process Engineering, Lisbon, Portugal, 16/05/2004 - 18/05/2004
reaction-separation-recycle, nonlinearity, integrated process design
DOI: 10.1016/S1570-7946(04)80144-5
Source: orbit
Source-ID: 135926
Publication: Research - peer-review › Article in proceedings – Annual report year: 2004

CAPEC overview and CAPE activities in Denmark
General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135894
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

CAPEC Research Report 2004
General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135961
Publication: Research › Report – Annual report year: 2004
Chemical Product Design: Challenges and Opportunities
This paper highlights for a class of chemical products, the design process, their design with respect to the important issues, the need for appropriate tools and finally, lists some of the challenges and opportunities for the process systems engineering (PSE)/computer-aided process engineering (CAPE) community. The chemical products considered belong to the following types: chemical/biochemical/agrochemical products, coatings and solvents, food (nutraceuticals), HIM (household, industrial and institutional), personal care, pharmaceuticals and drugs. The challenges and opportunities are highlighted in terms of the needs for multi-level modeling with emphasis on property models that are suitable for computer-aided applications, flexible solution strategies that are able to solve a large range of chemical product design problems and finally, a systems chemical product design framework with the overall objective to reduce the time and cost to market a new or improved product. (C) 2004 Elsevier Ltd. All rights reserved.
Scopus rating (2006): SJR 1.304 SNIP 1.936
Scopus rating (2005): SJR 1.314 SNIP 1.953
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.125 SNIP 1.908
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.348 SNIP 1.936
Scopus rating (2002): SJR 1.042 SNIP 0.92
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.955 SNIP 0.728
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.366 SNIP 1.025
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.073 SNIP 1.113
Original language: English
DOIs: 10.1016/j.compchemeng.2004.08.010
Source: orbit
Source-ID: 132427
Publication: Research - peer-review › Journal article – Annual report year: 2004

**Chemical Product Engineering: Product Analysis and Purification**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Publication date: 2004

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135875
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

**Computational algorithms for electrolyte system properties**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Takano, K. (Intern)
Pages: 371-404
Publication date: 2004

**Host publication information**
Title of host publication: Computer Aided Property Estimation for Process and Product Design
Volume: 19, Chapter 15
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 132410
Publication: Research - peer-review › Book chapter – Annual report year: 2004

**Computer-aided and predictive models for design of controlled release of pesticides**

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Suné, N. M. (Intern), Gani, R. (Intern)
Publication date: 2004

**Publication information**
Computer-aided and predictive models for design of controlled release of pesticides

In the field of pesticide controlled release technology, a computer based model that can predict the delivery of the Active Ingredient (AI) from fabricated units is important for purposes of product design and marketing. A model for the release of an M from a microcapsule device is presented in this paper, together with a specific case study application to highlight its scope and significance. The paper also addresses the need for predictive models and proposes a computer aided modelling framework for achieving it through the development and introduction of reliable and predictive constitutive models. A group-contribution based model for one of the constitutive variables (AI solubility in polymers) is presented together with examples of application and validation.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Suné, N. M. (Intern), Gani, R. (Intern)
Pages: 301-306
Publication date: 2004

Host publication information
Title of host publication: Proceedings of the 14th European Symposium on Computer Aided Process Engineering
Publisher: Elsevier Science
ISBN (Print): 0-444-51694-8
Series: Computer - Aided Chemical Engineering
Volume: 18
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 14th European Symposium on Computer Aided Process Engineering, Lisbon, Portugal, 16/05/2004 - 16/05/2004
controlled release, microcapsule, solubility prediction, pesticide, polymer
DOI: 10.1016/S1570-7946(04)80116-0
Source: orbit
Source-ID: 135928
Publication: Research - peer-review › Article in proceedings – Annual report year: 2004

Computer-aided and predictive models for design of controlled release of pesticides

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Suné, N. M. (Intern), Gani, R. (Intern)
Event: Poster session presented at Dansk Kemiingeniørkonference, Lyngby, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 154180
Publication: Research › Poster – Annual report year: 2004

Computer Aided Methods and Tools for Chemical Product Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Pages: 1494-1504
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Computer Aided Tools for Pesticide Formulation Products

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Munir, A. (Ekstern), Gani, R. (Intern)
Publication date: 2004

Design and Synthesis of Distillation Systems using a Driving Force Based Approach
A new integrated framework for synthesis, design and operation of distillation-based separation schemes is presented here. This framework is based on the driving force approach, which provides a measure of the differences in chemical/physical properties between two co-existing phases in a separation unit. A set of algorithms has been developed within this framework for design of simple as well as complex distillation columns, for the sequencing of distillation trains, for the determination of appropriate conditions of operation and for retrofit of distillation columns. The main feature of all these algorithms is that they provide a simple "visual" method to obtain near-optimal solutions in terms of energy consumption without rigorous simulation and/or optimisation. Several illustrative examples highlighting the application of the integrated approach are also presented. (C) 2003 Published by Elsevier B.V.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Bek-Pedersen, E. (Intern), Gani, R. (Intern)
Pages: 251-262
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering and Processing
Volume: 43
Issue number: 3
ISSN (Print): 0255-2701
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.766 SNIP 1.205 CiteScore 2.57
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.837 SNIP 1.389 CiteScore 2.63
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.87 SNIP 1.427 CiteScore 2.41
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.972 SNIP 1.391 CiteScore 2.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.017 SNIP 1.604 CiteScore 2.38
Design of Crystallization Solvents

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Achenie, L. (Ekstern), Karunanithi, A. T. (Ekstern), Gani, R. (Intern)
Publication date: 2004

Feasible operational paths serving as initial input for dynamic optimization

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Papaeconomou, E. (Intern), Jørgensen, S. B. (Intern)
Pages: 111-118
Publication date: 2004
Feasible operational paths serving as initial input for dynamic optimization

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Papaeeconomou, E. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 154098
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Generation of sustainable process (retrofit) alternatives through an indicator-based conflict resolution approach

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135878
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Group contribution based process flowsheet synthesis, design and modelling

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), d'Anterroches, L. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135879
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Group contribution based process flowsheet synthesis, design and modelling

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: d'Anterroches, L. (Intern), Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135891
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004
This paper presents a process-group-contribution Method to model, simulate and synthesize a flowsheet. The process-group based representation of a flowsheet together with a process “property” model are presented. The process-group based synthesis method is developed on the basis of the computer aided molecular design methods and gives the ability to screen numerous process alternatives without the need to use the rigorous process simulation models. The process “property” model calculates the design targets for the generated flowsheet alternatives while a reverse modelling method (also developed) determines the design variables matching the target. A simple illustrative example highlighting the main features of the methodology is also presented.
Modelling for Optimal Operation of Integrated Process Plant

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Papaeconomou, E. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), Cordiner, J. (Ekstern)
Publication date: 2004

Modelling of bioprocesses through a computer-aided modelling system

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2004

Nonlinear Behavior Analysis of Heat Integrated Distillation

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Pages: 691-696
Publication date: 2004

Nonlinear Behaviour Analysis for Design and Operation of Copolymerization Reactors

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sales-Cruz, A. M. (Intern), Lopez-Arenas, M. T. (Intern), Gani, R. (Intern)
Optimal (solvent) mixture design through a decomposition based CAMD methodology

Computer Aided Molecular/Mixture design (CAMD) is one of the most promising techniques for solvent design and selection. A decomposition based CAMD methodology has been formulated where the mixture design problem is solved as a series of molecular and mixture design sub-problems. This approach is able to overcome most of the difficulties associated with the solution of mixture design problems. The new methodology has been illustrated with the help of a case study involving the design of solvent-anti solvent binary mixtures for crystallization of Ibuprofen.

Optimal (Solvent) Mixture Design through a Decomposition Based CAMD methodology

Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Karunanithi, A. T. (Ekstern), Achenie, L. (Ekstern), Gani, R. (Intern)
Published: 2004
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Achenie, L. (Ekstern), Karunanithi, A. T. (Ekstern), Gani, R. (Intern)
Pages: 217-222
Publication date: 2004

Host publication information
Title of host publication: European Symposium on Computer Aided Process Engineering - 14
Publisher: Elsevier Science
ISBN (Print): 0-444-51694-8, 978-0-444-51694-7

Series: Computer - Aided Chemical Engineering
Volume: 18
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
Conference: 14th European Symposium on Computer Aided Process Engineering, Lisbon, Portugal, 16/05/2004 - 16/05/2004
CAMD, MINLP, Optimization, Mixture design, Solvents, Ibuprofen
Electronic versions:
1_s2.0_S1570794604801020_main.pdf
DOIs:
10.1016/S1570-7946(04)80102-0
Source: orbit
Source-ID: 135931
Publication: Research - peer-review › Article in proceedings – Annual report year: 2004

Optimizing control of a heat integrated distillation pilot plant

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 154361
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Optimizing Control of Heat Integrated Distillation Pilot Plant

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135900
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Part II: Models for Properties

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Abildskov, J. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 436
Publication date: 2004
Part I. Introduction to Computer Aided Property Estimation

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Gani, R. (Intern), Kontogeorgis, G. (Intern)
Number of pages: 436
Publication date: 2004

Host publication information
Title of host publication: Computer Aided Property Estimation for Process and Product Design
Publisher: Elsevier
ISBN (Print): 978-0-444-51153-9
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209328
Publication: Research - peer-review › Book chapter – Annual report year: 2004

Part IV: Challenges and Opportunities

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 436
Publication date: 2004

Host publication information
Title of host publication: Computer Aided Property Estimation for Process and Product Design
Publisher: Elsevier
ISBN (Print): 978-0-444-51153-9
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209180
Publication: Research - peer-review › Book chapter – Annual report year: 2004

Predictive property models for use in design of controlled release of pesticides

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Suné, N. M. (Intern), Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135886
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004
Property cluster based visual technique for synthesis and design of formulations

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Eden, M. R. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), El-Halwagi, M. M. (Ekstern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135914
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Property models in computation of phase equilibrium

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Gani, R. (Intern), Kontogeorgis, G. (Intern)
Pages: 309-338
Publication date: 2004

Host publication information
Title of host publication: Computer Aided Property Estimation for Process and Product Design
Volume: 19, Chapter 13
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 132409
Publication: Research - peer-review › Book chapter – Annual report year: 2004

Pure component property estimation: Models & databases

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Morejon, J. M. (Intern), Gani, R. (Intern)
Pages: 45-58
Publication date: 2004

Host publication information
Title of host publication: Computer Aided Property Estimation for Process and Product Design
Volume: 19, Chapter 3
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 132405
Publication: Research - peer-review › Book chapter – Annual report year: 2004

Reverse problem formulation based techniques for process-product synthesis and design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Eden, M. R. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), El-Halwagi, M. M. (Ekstern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Role of properties and their models in process and product design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), O'Connell, J. (Ekstern)
Pages: 27-42
Publication date: 2004

Host publication information
Title of host publication: Computer Aided Property Estimation For Porcess and Product Design
Volume: 19, Chapter 2
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 132400
Publication: Research - peer-review › Book chapter – Annual report year: 2004

Short-Path Separation Schemes for Chemical Product Modeling, Analysis and Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Sales-Cruz, A. M. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135873
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

Systematic generation and evaluation of sustainable process alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Jørgensen, S. B. (Intern), Davidescu, F. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135902
Publication: Research › Sound/Visual production (digital) – Annual report year: 2004

The reverse approach for synthesis and design of products and processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 135893
Thermodynamic method for obtaining the solubilities of complex medium-sized chemicals in pure and mixed solvents

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Abildskov, J. (Intern), Gani, R. (Intern)
Publication date: 2004

Property Based Process and Product Synthesis and Design
This thesis describes the development of a general framework for solving process and product design problems. Targeting the desired performance of the system in a systematic manner relieves the iterative nature of conventional design techniques. Furthermore, conventional component based methods are not capable of handling problems, where the process or product objectives are driven by functionalities or properties rather than chemical constituency. The framework is meant to complement existing composition based methods by being able to handle property driven problems. By investigating the different roles a property model plays at different stages of the solution to a design problem, it is discovered that by decoupling the constitutive equations, that make up the property model, from the balance and constraint equations of the process or product model, a significant reduction in problem complexity is achieved including an added flexibility compared to existing solution methods. The decoupling of the constitutive equations allows for reformulating a conventional forward problem into two reverse problems. The first reverse problem is the reverse of a simulation problem, where the process model is solved in terms of the constitutive (synthesis/design) variables instead of the process variables, thus providing the synthesis/design targets. The second reverse problem (reverse property prediction) solves the constitutive equations to identify unit operations, operating conditions and/or products by matching the synthesis/design targets. The reverse problem formulation technique extends the application range of the numerical solvers as well as the models themselves, thus it is possible to identify alternative designs that conventional methods are not capable of finding. A novel way of representing the constitutive variables is presented in this thesis. The framework is based on tracking functionalities or properties of the process streams rather than the chemical constituency. The motivation for developing this framework comes from a number of cases where conventional composition based methods fail to adequately solve the design problems. The methodology for tracking stream functionalities or properties is referred to as property clustering. The clusters are derived to obey the principles of intra- and interstream conservation, which allow for the development of consistent additive rules along with their ternary representation, thereby facilitating visualization on triangular diagrams. An important feature of the clustering technique is the ability to reduce a high dimensional problem into a two or three dimensional space allowing for visualization of the problem. The developed framework provides a systematic methodology for solving process and product design problems. The reverse problem formulation techniques allow for easier identification of optimal solutions and the property clustering techniques enable the systematic solution of problems that are driven by physical properties rather than components. It should be emphasized that the work presented here introduces the general framework of reverse problem formulation, where the links between the two formulated reverse problems are the constitutive variables. One representation of such variables is the property clustering methodology presented here, but the general framework is applicable to any representation of the properties.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Eden, M. R. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Publication date: Dec 2003

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Source: orbit
Source-ID: 41328
Publication: Research › Ph.D. thesis – Annual report year: 2003
A conceptual "Design" Based Method for Generation of Batch Recipes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Papaeconomou, E. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), Cordiner, J. (Ekstern)
Publication date: 2003

Host publication information
Title of host publication: Proceedings of FOCAPO 2003, Florida, USA
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 154097
Publication: Research › Article in proceedings – Annual report year: 2003

A Modelling Tool for Different Stages of the Process Life

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Sales-Cruz, A. M. (Intern), Gani, R. (Intern)
Pages: 209-237
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Dynamic Model Development: Methods, Theory and Application
Volume: 0
Issue number: 0
Original language: English
Source: orbit
Source-ID: 41151
Publication: Research - peer-review › Journal article – Annual report year: 2003

Analysis of Optimal Operation of an Energy Integrated Distillation Plant

The efficiency of manufacturing systems can be significantly increased through diligent application of control based on mathematical models thereby enabling more tight integration of decision making with systems operation. In the present paper analysis of optimal operation of an energy integrated distillation plant is investigated more closely with the purpose of elucidating essential decisions behind planning experiments, which are suitable for identifying models and constraints. The basis for analysis of optimal operation is the type of operation upon which an application focuses. In this paper the attention is on achieving close to optimal economical benefit of a continuously operating plant. The optimal operation region for the plant is visualized by the profit landscape of the example process. The nonlinear dynamic behavior within the optimal operation region is studied through bifurcation analysis. Thereafter a series of decisions have to be made concerning the experimental design for revealing the plant steady states and dynamics within the optimal operating region. However in this paper the focus is upon revealing the possible nonlinear behaviors around the optimal operating region and their influence upon the further decisions behind the experimental design. An energy-integrated distillation column, which may exhibit fold bifurcations, is used as a relevant example process.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Li, H. W. (Intern), Hansen, C. (Ekstern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Pages: 940-945
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Computer - Aided Chemical Engineering
Volume: 15
Issue number: part A-B
ISSN (Print): 1570-7946
Ratings:
BFI (2017): BFI-level 1
A New Modeling Approach for Future Challenges in Process and Product Design

In this paper, a new technique for model reduction that is based on rearranging a part of the model representing the constitutive equations is presented. The rearrangement of the constitutive equations leads to the definition of a new set of pseudo-intensive variables, where the component compositions are replaced by reduction parameters in the process model. Since the number of components dominates the size of the traditional model equations, a significant reduction of the model size is obtained through this new technique. Some interesting properties of this new technique is that the model reduction does not introduce any approximations to the model, it does not change the physical location of the process variables and it provides a visualization of the process and operation that otherwise would not be possible. Furthermore by employing the recently introduced principle of reverse problem formulations, the solution of integrated process/product design problem becomes simpler and more flexible.
A New Modeling Approach for Future Challenges in Process and Product Design

In this paper, a new technique for model reduction that is based on rearranging a part of the model representing the constitutive equations is presented. The rearrangement of the constitutive equations leads to the definition of a new set of pseudo-intensive variables, where the component compositions are replaced by reduction parameters in the process model. Since the number of components dominates the size of the traditional model equations, a significant reduction of the model size is obtained through this new technique. Some interesting properties of this new technique is that the model reduction does not introduce any approximations to the model, it does not change the physical location of the process variables and it provides a visualisation of the process and operation that otherwise would not be possible. Furthermore by employing the recently introduced principle of reverse problem formulations, the solution of integrated process/product design problem becomes simpler and more flexible.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Eden, M. R. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern)
Pages: 101-106
Publication date: 2003

Host publication information
Title of host publication: European Symposium on Computer Aided Process Engineering - 13
Volume: 14
Publisher: Elsevier Science
ISBN (Print): 0-444-51368-X
Series: Computer - Aided Chemical Engineering
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
DOIs: 10.1016/S1570-7946(03)80098-6
Source: orbit
Source-ID: 153944
Publication: Research - peer-review › Article in proceedings – Annual report year: 2003

A New Screening Methodology for the Identification of Economically Beneficial Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Hungerbühler, K. (Ekstern), Fischer, U. (Ekstern)
Pages: 2400-2418
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: AIChE Journal
Volume: 49
Issue number: 9
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
An Integrated Computer Aided System for Generation and Evaluation of Sustainable Process Alternatives

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Jensen, N. (Intern), Coll, N. (Ekstern), Gani, R. (Intern)
Pages: 209-225
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Clean Technologies & Environmental Policies
Volume: 5
Graphical and State-to-State Methods for Reactive Distillation Column Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sanchez Daza, O. (Ekstern), Bek-Pedersen, E. (Intern), Perez-Cisneros, E. (Ekstern), Gani, R. (Intern)
Pages: 2822-2841
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: AIChE Journal
Volume: 49
Issue number: 11
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Process Flowsheet Generation and Design through a Group- Contribution Approach Features

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2003

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40916
Publication: Research › Sound/Visual production (digital) – Annual report year: 2003
Property Cluster based Visual Technique for Synthesis and Design of Formulation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Eden, M. R. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), El-Halwegi, M. (Ekstern)
Pages: 1175-1180
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Computer - Aided Chemical Engineering
Volume: 15B
ISSN (Print): 1570-7946
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.198 SNIP 0.215 CiteScore 0.48
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.245 SNIP 0.249 CiteScore 0.39
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.239 SNIP 0.217 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.216 SNIP 0.175 CiteScore 0.28
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.196 SNIP 0.267 CiteScore 0.33
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.194 SNIP 0.199 CiteScore 0.3
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.181 SNIP 0.135
Scopus rating (2009): SJR 0.16 SNIP 0.163
Scopus rating (2008): SJR 0.167 SNIP 0.124
Scopus rating (2007): SJR 0.182 SNIP 0.094
Scopus rating (2006): SJR 0.138 SNIP 0.108
Scopus rating (2005): SJR 0.178 SNIP 0.178
Scopus rating (2004): SJR 0.19 SNIP 0.161
Scopus rating (2003): SJR 0.157 SNIP 0.212
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.168 SNIP 0.214
Scopus rating (2001): SJR 0.146 SNIP 0.193
Reverse Problem Formulation Based Techniques for Process and Synthesis and Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Eden, M. R. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), El-Halwagi, M. (Ekstern)
Pages: 451-456
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Computer - Aided Chemical Engineering
Volume: 15B
ISSN (Print): 1570-7946
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.198 SNIP 0.215 CiteScore 0.48
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.245 SNIP 0.249 CiteScore 0.39
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.239 SNIP 0.217 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.216 SNIP 0.175 CiteScore 0.28
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.196 SNIP 0.267 CiteScore 0.33
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.194 SNIP 0.199 CiteScore 0.3
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.181 SNIP 0.135
Scopus rating (2009): SJR 0.16 SNIP 0.163
Scopus rating (2008): SJR 0.167 SNIP 0.124
Scopus rating (2007): SJR 0.182 SNIP 0.094
Scopus rating (2006): SJR 0.138 SNIP 0.108
Scopus rating (2005): SJR 0.178 SNIP 0.178
Scopus rating (2004): SJR 0.19 SNIP 0.161
Scopus rating (2003): SJR 0.157 SNIP 0.212
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.168 SNIP 0.214
Scopus rating (2001): SJR 0.146 SNIP 0.193
Scopus rating (2000): SJR 0.102 SNIP 0
Scopus rating (1999): SJR 0.102 SNIP 0
Original language: English
Source: orbit
Source-ID: 153949
Publication: Research - peer-review › Conference article – Annual report year: 2003

Synthesis and Design of Distillation based Separation Schemes
Integrated Approach to Computer Aided Process Synthesis

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Hostrup, M. (Intern), Gani, R. (Intern)
Publication date: Apr 2002

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: PEC02-07.pdf
Source: orbit
Source-ID: 40897
Publication: Research › Ph.D. thesis – Annual report year: 2002

A conceptual "Design" Based Method for Generation of Batch Recipes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Papaeconomou, E. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), Cordiner, J. (Ekstern)
Publication date: 2002

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41432
Publication: Research › Sound/Visual production (digital) – Annual report year: 2002

A Framework Towards the Optimal Sequencing and Operational Modelling of Batch Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Papaeconomou, E. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern)
Publication date: 2002

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41054
Publication: Research › Sound/Visual production (digital) – Annual report year: 2002

A Framework towards the Optimal Synthesis and Operational Modelling of Batch Processes

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Papaeconomou, E. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern)
Publication date: 2002

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
A general framework for the synthesis and operational design of batch processes
The objective of this paper is to present a general problem formulation and a general methodology for the synthesis of batch operations and the operational design of individual batch processes, such as mixing, reaction and separation. The general methodology described supplies the batch routes, which is the sequence of batch operations performed in order to achieve a specific objective. Important features of the methodology are a set of rule-based algorithms that provide the operational model of the units. Such an algorithm is highlighted, together with the associated rules, for the operational design of batch reactors. A case study involving the feasible operation of a batch reactor with multiple desirable and undesirable reactions and operational constraints is presented. Application results including verification of the generated operational sequences (alternatives) through dynamic simulation are presented.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Papaeconomou, E. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Pages: 289-294
Publication date: 2002

Host publication information
Title of host publication: EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING - 12
Volume: 10
ISBN (Print): 0-444-51109-1
Series: Computer - Aided Chemical Engineering
Volume: 10
ISSN: 1570-7946
Main Research Area: Technical/natural sciences
DOIs: 10.1016/S1570-7946(02)80076-1
Source: orbit
Source-ID: 40904
Publication: Research - peer-review › Article in proceedings – Annual report year: 2002

A General framework for the Synthesis and Operational Design of Batch Processes
The objective of this paper is to present a general problem formulation and a general methodology for the synthesis of batch operations and the operational design of individual batch processes, such as mixing, reaction and separation. The general methodology described supplies the batch routes, which is the sequence of batch operations performed in order to achieve a specific objective. Important features of the methodology are a set of rule-based algorithms that provide the operational model of the units. Such an algorithm is highlighted, together with the associated rules, for the operational design of batch reactors. A case study involving the feasible operation of a batch reactor with multiple desirable and undesirable reactions and operational constraints is presented. Application results including verification of the generated operational sequences (alternatives) through dynamic simulation are presented.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center
Authors: Papaeconomou, E. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern)
Publication date: 2002

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41049
Publication: Research › Sound/Visual production (digital) – Annual report year: 2002

A Novel Technique for Process Model Reduction

General information
Blanket Wash Solvent Blend Design using Interval Analysis

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Sinha, M. (Ekstern), Achenie, L. (Ekstern), Gani, R. (Intern)
Pages: 516-527
Publication date: 2002
Main Research Area: Technical/natural sciences
Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 42
Issue number: 0
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
Computer Aided Modelling of Pesticide Uptake in Plants for Pesticide Formulation and Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Suné, N. M. (Intern), Gani, R. (Intern), Bell, G. (Ekstern), Cordiner, J. (Ekstern)
Publication date: 2002

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41024
Publication: Research - peer-review › Journal article – Annual report year: 2002

Computer-Aided Methods and Tools for the Pharmaceutical Industry

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2002

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41074
Publication: Research › Sound/Visual production (digital) – Annual report year: 2002

Computer Aided Model Analysis and Dynamic Simulation of Wastewater Treatment Plant
Computer Aided System for Creating problem Specific Property Models

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Kang, J. W. (Intern), Gani, R. (Intern)
Publication date: 2002

Publication information
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41057
Publication: Research - peer-review › Journal article – Annual report year: 2002

Conceptual design and analysis methodology for crystallization processes with electrolyte systems

General information
State: Published
Design and Synthesis of Separation Systems Using a Driving Force Approach

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Bek-Pedersen, E. (Intern), Gani, R. (Intern)
Publication date: 2002

**Publication information**

Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40865
Publication: Research - peer-review › Journal article – Annual report year: 2002

Estimation of Mixture Properties from first and second-order group contributions with UNIFAC models

**General information**

State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Kang, J. W. (Intern), Abildskov, J. (Intern), Gani, R. (Intern), Cobos, J. (Ekstern)
Pages: 3260-3273
Publication date: 2002
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Industrial & Engineering Chemistry Research
Volume: 14
Issue number: 13
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
Group Contribution Based Estimation of Octanol/Water Partition Coefficient and Aqueous Solubility

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Morejon, J. M. (Intern), Gani, R. (Intern)
Pages: 6623-6633
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 41
Issue number: 25
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.342 SNIP 1.398
Original language: English
Source: orbit
Source-ID: 40844
Publication: Research - peer-review › Journal article – Annual report year: 2002

ICAS Integrated Computer Aided System for Education

General information
Identifying Process and Product Synthesis Targets by Reverse Problem Formulation Techniques

Integration of Design and Control for Energy Integrated Distillation
Integration of Design and Control through Model Analysis

A systematic computer aided analysis of the process model is proposed as a pre-solution step for integration of design and control problems. The process model equations are classified in terms of balance equations, constitutive equations and conditional equations. Analysis of the phenomena models representing the constitutive equations identify the relationships between the important process and design variables, which help to understand, define and address some of the issues related to integration of design and control. Furthermore, the analysis is able to identify a set of process (control) variables and design (manipulative) variables that may be employed with different objectives in design and control for the integrated problem. The computer aided model analysis is highlighted through illustrative examples, involving processes with mass and/or energy recycle, where the important design and control (structure selection) issues for the integrated problems are considered. (C) 2002 Elsevier Science Ltd. All rights reserved.
Nanotechnology at KT

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Membrane Technology group, Center for Phase Equilibria and Separation Processes, Computer Aided Process Engineering Center
Authors: Glarborg, P. (Intern), Hassager, O. (Intern), Jonsson, G. E. (Intern), Stenby, E. H. (Intern), Gani, R. (Intern)
Publication date: 2002

Optimal Mixture Design Through an Extended CAMD Technique

General information
Performance Analysis of Denitrifying Wastewater Treatment Plants

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Mussati, M. (Ekstern), Gernaey, K. (Intern), Gani, R. (Intern), Jørgensen, S. B. (Intern)
Pages: 171-182
Publication date: 2002
Main Research Area: Technical/natural sciences
Publication information
Journal: Clean Technologies & Environmental Policies
Volume: 4
Issue number: 0
Original language: English
Source: orbit
Source-ID: 40775
Publication: Research - peer-review › Journal article – Annual report year: 2002

Property Integration - A New Approach for Simultaneous Solution of Process and Molecular Design Problems

The objective of this paper is to introduce the new concept of property integration. It is based on tracking and integrating properties throughout the process. This is made possible by exploiting the unique features at the interface of process and molecular design. Recently developed clustering concepts are employed to identify optimal properties without commitment to specific species. Subsequently, group contribution methods and molecular design techniques are employed to solve the reverse property prediction problem to design molecules possessing the optimal properties.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Eden, M. R. (Intern), Jørgensen, S. B. (Intern), Gani, R. (Intern), El-Halwagi, M. M. (Ekstern)
Publication date: 2002

Property Modelling and Simulation for Product and Process Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern), Pistikopoulos, S. (Ekstern)
Pages: 43-59
Publication date: 2002
Main Research Area: Technical/natural sciences
Research at KT 2002

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering
Authors: Glarborg, P. (Intern), Hassager, O. (Intern), Jonsson, G. E. (Intern), Stenby, E. H. (Intern), Gani, R. (Intern)
Publication date: 2002

Roles of Modeling in Process/Product Synthesis & Design for Sustainable Development

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2002

Software Architectures and Tools for Computer Aided Process Engineering

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Braunschweig, B. (Ekstern), Gani, R. (Intern)
Publication date: 2002

Solvent Selection in Chemical Engineering by Molecular Design

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2002
Targetted development of appropriate technology with low CO2 consumption

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Jørgensen, S. B. (Intern), Eden, M. R. (Intern), Gani, R. (Intern)
Publication date: 2002

**Publication information**
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences

**Bibliographical note**
Presented by Sten Bay Jørgensen
Source: orbit
Source-ID: 40769
Publication: Research › Sound/Visual production (digital) – Annual report year: 2002

The Age of Computer Aided Modelling

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Gani, R. (Intern)
Publication date: 2002

**Publication Information**
Original language: English
Volume: 0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41053
Publication: Research › Sound/Visual production (digital) – Annual report year: 2002

The interactions of design, control and operability in reactive distillation systems

In this work the design and control of a reactive distillation column, described by a rigorous dynamic model, is tackled via two different optimization approaches. In the first, the steady-state process design and the control system are optimized sequentially. It is shown that operability is a strong function of the process design and potential operability bottlenecks are identified. In the second approach, the process design and the control system are optimized simultaneously leading to a more economically beneficial and better controlled system than that obtained using the sequential approach. (C) 2002 Elsevier Science Ltd. All rights reserved.

**General information**
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Authors: Georgiadis, M. (Ekstern), Schenk, M. A. (Ekstern), Pistikopoulos, S. (Ekstern), Gani, R. (Intern)
Pages: 735-746
Publication date: 2002

**Publication information**
Journal: Computers & Chemical Engineering
Volume: 26
Issue number: 4
ISSN (Print): 0098-1354
Ratings:
Projects:

**Solvent Molecular Design Process Synthesis and Energy Requirements in Chemical and Biochemical Processes**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2017 → 31/10/2020  
Number of participants: 4  
PhD Student:  
Chen, Yuqiu (Ekstern)  
Supervisor:  
Gani, Rafiqul (Intern)  
Kontogeorgis, Georgios (Intern)  
Main Supervisor:  
Woodley, John (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Stipendie fra udlandet  
Project: PhD

**Chemical & Biochemical Sustainable Process Synthesis - Intensification**

Department of Chemical and Biochemical Engineering  
Period: 15/10/2016 → 14/10/2019  
Number of participants: 4  
PhD Student:  
Garg, Nipun (Intern)  
Supervisor:  
Gani, Rafiqul (Intern)  
Kontogeorgis, Georgios (Intern)  
Main Supervisor:  
Woodley, John (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansierede - Virksomhed  
Project: PhD

**Models for estimation and analyses of emissions from chemical processes and products**

Department of Chemical and Biochemical Engineering
Period: 01/10/2016 → 30/09/2019
Number of participants: 5
Phd Student:
Jhamb, Spardha Virendra (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Kontogeorgis, Georgios (Intern)
Liang, Xiaodong (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Energy Efficiency Hybrid Separation Process with Ionic Liquid
Department of Chemical and Biochemical Engineering
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Liu, Xinyan (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Liang, Xiaodong (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Systematic computer aided methods and tools for lipids process technology
Department of Chemical and Biochemical Engineering
Period: 15/09/2015 → 14/09/2018
Number of participants: 5
Phd Student:
Ana Perederic, Olivia (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Kontogeorgis, Georgios (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Woodley, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Sustainable process design with process intensification
Department of Chemical and Biochemical Engineering
Period: 01/10/2014 → 14/12/2017
Number of participants: 6
Phd Student:
Frauzem, Rebecca (Intern)
Supervisor:
Advanced thermodynamic cycles utilising low-temperature heat sources

Energy sources at a low temperature level are available from a variety of sources ranging from waste heat from ships, industry and refrigeration plants, to renewable energy in the form of biomass, geothermal and solar.

There is significant potential for improving the use of these sources in developing new cycles based on new multi-component fluid mixtures. These improvements will not only increase the efficiency of today's technology, but they will also make it possible to use low-temperature sources which, due to lack of technical feasibility or economy is not used today. This ambitious, interdisciplinary project will lead the way to innovative thermal system for electricity generation, heat pumping and cooling by utilization of low value sources, at efficiencies that surpasses today's level significantly. The project will develop advances in the design of both processes and media so that energy savings of 15% can be achieved. The analysis will include numerical simulation and advanced thermodynamic methods based on energy and exergy analysis and experimental verification of component performance. The development of a systematic approach to the optimization of cycle and the working medium in the given application. The results will provide a scientific basis for choosing the future use of low-temperature resources in Denmark. This may contribute significantly to the development of the future society using no fossil resources, but large amounts of fluctuating renewable energy.

Department of Mechanical Engineering
Thermal Energy
Department of Chemical and Biochemical Engineering
CAPEC-PROCESS
Danish Technological Institute
Danfoss A/S
Viegand Maagøe
Alfa Laval
MAN Diesel & Turbo SE
A. P. Møller-Mærsk
Arla Foods
Technical University of Munich
Delft University of Technology
Aalborg University
Alfa Laval
Period: 01/03/2014 → 28/02/2019
Number of participants: 17
Acronym: THERMCYC
Project ID: 76567
Number of related Ph.D. students: 7
Project participant:
Haglind, Fredrik (Intern)
Clausen, Lasse Røngaard (Intern)
Kærn, Martin Ryhl (Intern)
Markussen, Wiebke Brix (Intern)
Sin, Gürkan (Intern)
Gani, Rafiqul (Intern)
Babi, Deenesh Kavi (Intern)
Pierobon, Leonardo (Intern)
Zhang, Lei (Intern)
Zühlsdorf, Benjamin (Intern)
Mancini, Roberta (Intern)
Phd Student:
Meroni, Andrea (Intern)
Andreasen, Jesper Graa (Intern)
Cignitti, Stefano (Intern)
Frutiger, Jerome (Intern)
Project Manager, academic:
Elmegaard, Brian (Intern)
Project Coordinator:
Sørensen, Iben (Intern)

Relations
Activities:
International Workshop on High Temperature Heat Pumps
Publications:
Mapping of low temperature heat sources in Denmark
Improving efficiency of heat pumps by use of zeotropic mixtures for different temperature glides
Book of presentations of the International Workshop on High Temperature Heat Pumps
Project report: Experimental planning and verification of working fluids (WP 5)
Industrial Energy Mapping: THERMCYC WP6
High Temperature Heat Pump Integration using Zeotropic Working Fluids for Spray Drying Facilities
Forbedring af industrielle processers energieffektivitet
Derivation of guidelines for the design of plate evaporators in heat pumps using zeotropic mixtures

Improved LCA Methodology and software tool for biorenewable products and processes
Department of Chemical and Biochemical Engineering
Period: 15/12/2013 → 25/01/2017
Number of participants: 6
Phd Student:
Kumar Tula, Anjan (Intern)
Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Woodley, John (Intern)
Harper, Peter Mathias (Intern)
Manenti, Flavio (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)

Relations
Publications:
Computer-Aided Sustainable Process Synthesis-Design and Analysis
Project: PhD

Modeling and Synthesis of Pharmaceutical processes: Moving from Batch to Continuous Manufacturing

Department of Chemical and Biochemical Engineering
Period: 01/10/2013 → 16/11/2016
Number of participants: 7
Phd Student:
Papadakis, Emmanouil (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Eden, Mario Richard (Intern)
Eden, Mario Richard (Intern)
Jiménez-González, Concepción (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Modelling and synthesis of pharmaceutical processes: moving from batch to continuous
Project: PhD

Design, control and analysis of intensified biochemical processes

Department of Chemical and Biochemical Engineering
Period: 01/09/2013 → 16/11/2016
Number of participants: 7
Phd Student:
Mansouri, Seyed Soheil (Intern)
Supervisor:
Huusom, Jakob Kjøbsted (Intern)
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
von Solms, Nicolas (Intern)
Lee, Jay Hyung (Ekstern)
Ricardez-Sandoval, Luis (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

**Relations**
Publications:
Integrated Process Design, Control and Analysis of Intensified Chemical Processes
Project: PhD

**Generic model-based tailor-made design and analysis of biphasic reacting systems**
Department of Chemical and Biochemical Engineering
Period: 01/08/2013 → 24/10/2016
Number of participants: 6
Phd Student:
Anantpinjiwatna, Amata (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Huusom, Jakob Kjøbsted (Intern)
Grosjean, Christophe (Ekstern)
Manenti, Flavio (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet

**Relations**
Publications:
Generic Model-Based Tailor-Made Design and Analysis of Biphasic Reaction Systems
Project: PhD

**Property Modelling and Process Design involving complex chemical systems**
Department of Chemical and Biochemical Engineering
Period: 01/06/2013 → 18/08/2016
Number of participants: 7
Phd Student:
Kalakul, Sawitree (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Woodley, John (Intern)
Achenie, Luke E. K. (Ekstern)
Jiménez-González, Concepción (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

**Relations**
Publications:
Property Model-based Tailor-made Design of Chemical-based Products
**Systematic Methods and Tools for Computer Aided Modeling**

Department of Chemical and Biochemical Engineering  
Period: 01/04/2012 → 02/09/2015  
Number of participants: 6  
Phd Student:  
Fedorova, Marina (Intern)  
Supervisor:  
Sin, Gürkan (Intern)  
Main Supervisor:  
Gani, Rafiqul (Intern)  
Examiner:  
Gernaey, Krist V. (Intern)  
Linninger, Andreas A. (Ekstern)  
Preisig, Heinz A. (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Anden EU-finansiering  
Project: PhD

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**Modelling of phase equilibria and related properties of mixtures involving lipids**

Department of Chemical and Biochemical Engineering  
Period: 01/02/2012 → 13/05/2015  
Number of participants: 6  
Phd Student:  
Cunico, Larissa (Intern)  
Supervisor:  
Sarup, Bent (Ekstern)  
Main Supervisor:  
Gani, Rafiqul (Intern)  
Examiner:  
Kontogeorgis, Georgios (Intern)  
Sales Cruz, Alfonso Mauricio (Intern)  
Jaubert, Jean-Noël (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet  
Project: PhD

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**Phenomena based process intensification**

Department of Chemical and Biochemical Engineering  
Period: 01/09/2011 → 04/02/2015  
Number of participants: 6  
Phd Student:  
Babi, Deenesh Kavi (Intern)  
Supervisor:  
Woodley, John (Intern)  
Main Supervisor:  
Gani, Rafiqul (Intern)  
Examiner:  
Huusom, Jakob Kjøbsted (Intern)  
Sundmacher, Kai (Ekstern)  
Van Gerven, Tom (Ekstern)
Systematic methodology for design of emulsion based chemical products

Department of Chemical and Biochemical Engineering
Period: 01/08/2011 → 30/09/2014
Number of participants: 6
PhD Student:
Mattei, Michele (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Kate, Antoon J. B. ten (Ekstern)
Wiebe, Lars (Ekstern)

A methodology for systematic design and selection of green solvents for increased yield in organic reactions

Department of Chemical and Biochemical Engineering
Period: 01/11/2010 → 31/03/2013
Number of participants: 4
PhD Student:
Mitrofanov, Igor (Intern)
Supervisor:
Abildskov, Jens (Intern)
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
**Financing sources**
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

**Tailor-made design of chemical products: Bio-fuels and other blended products**
Department of Chemical and Biochemical Engineering
Period: 15/07/2010 → 07/05/2014
Number of participants: 7
Phd Student:
Yunus, Nor Alafiza Binti (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Sin, Gürkan (Intern)
Harper, Peter Mathias (Intern)
Kate, Antoon J. B. ten (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

**Model Based Integrated Process-Product Design - retrofitting and optimisation**
Department of Chemical and Biochemical Engineering
Period: 01/07/2010 → 30/09/2013
Number of participants: 8
Phd Student:
Hukkerikar, Amol Shivajirao (Intern)
Supervisor:
Abildskov, Jens (Intern)
Gani, Rafiqul (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Frenkel, Michael (Ekstern)
Krooshof, Gerard (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

**Incremental refinement of process design**
Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 30/09/2013
Number of participants: 7
Phd Student:
Quaglia, Alberto (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Sarup, Bent (Ekstern)
Main Supervisor:
Sin, Gürkan (Intern)
Examiner:
Jørgensen, John Bagterp (Intern)
Bode, Andreas (Ekstern)
Pistikopoulos, Efstratios N. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Modelling controlled release of substrate and removal of products in biocatalysis
Department of Chemical and Biochemical Engineering
Period: 01/11/2009 → 21/05/2013
Number of participants: 7
Phd Student:
Al-Haque, Naweed (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Tufvesson, Pär (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Krühne, Ulrich (Intern)
Daugulis, Andrew J. (Ekstern)
Spiess, Antje C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

New Product Start Up in Pharmaceutical Production
Department of Management Engineering
Period: 01/09/2009 → 21/02/2014
Number of participants: 8
Phd Student:
Hansen, Klaus Reinholdt Nyhuus (Intern)
Supervisor:
Akkerman, Renzo (Intern)
Gani, Rafiqul (Intern)
Grunow, Martin (Intern)
Main Supervisor:
Hvam, Lars (Intern)
Examiner:
Jacobsen, Peter (Intern)
Jósef, Váncza (Ekstern)
Olhager, Jan Erik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Development and Analysis of Group-Constribustion plus Models for Property Prediction of Organic Chemical Systems
Department of Chemical and Biochemical Engineering
Period: 01/04/2009 → 19/03/2013
Number of participants: 6
Phd Student:
Mustaffa, Azizul Azri (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Abildskov, Jens (Intern)
Voutsas, Epaminondas C. (Ekstern)
Wiebe, Lars (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

**Control of Process Operations and Monitoring of Product Qualities through Hybrid Multi-Scale Model-Based Analysis**
Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 21/11/2012
Number of participants: 7
Phd Student:
Abdul Samad, Noor Asma Fazli Bin (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, John Bagterp (Intern)
Georgiadis, Michael C. (Ekstern)
Kalman Nagy, Zoltan (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

**Computer-aided modelling for efficient and innovative product-process engineering**
Department of Chemical and Biochemical Engineering
Period: 01/12/2008 → 18/04/2012
Number of participants: 7
Phd Student:
Heitzig, Martina (Intern)
Supervisor:
Glarborg, Peter (Intern)
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Piccione, Patrick M. (Ekstern)
Pistikopoulos, Stratos (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Green Chemistry based innovative process-operation synthesis and design
Department of Chemical and Biochemical Engineering
Period: 01/12/2008 → 18/04/2012
Number of participants: 6
Phd Student:
Lutze, Philip (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Woodley, John (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Berg, Henk van den (Ekstern)
Freund, Hannsjörg (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Optimization of Tailor-made Chemicals from Renewable and non-renewable sources
Department of Chemical and Biochemical Engineering
Period: 01/09/2008 → 01/02/2010
Number of participants: 4
Phd Student:
Swangkotchakorn, Chutima (Intern)
Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Moving from batch towards continuous organic-chemical pharmaceutical production
Department of Chemical and Biochemical Engineering
Period: 01/08/2008 → 08/02/2012
Number of participants: 8
Phd Student:
Cervera Padrell, Albert Emili (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Kiil, Søren (Intern)
Skovby, Tommy (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Jensen, Anker Degn (Intern)
Aelterman, Wim (Ekstern)
Hartman, Ryan L. (Ekstern)

Financing sources
Source: Internal funding (public)
Systematic Modelling, Simulation and Design of Intensified Bio-Chemical Processes

Department of Chemical and Biochemical Engineering
Period: 01/08/2008 → 29/11/2011
Number of participants: 6
PhD Student:
Roman Martinez, Alicia (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Sales Cruz, Alfonso Mauricio (Intern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Computer Modelling of Lipid Processing Technology

Department of Chemical and Biochemical Engineering
Period: 01/05/2008 → 29/11/2011
Number of participants: 6
PhD Student:
Diaz Tovar, Carlos Axel (Intern)
Supervisor:
Sarup, Bent (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Sin, Gürkan (Intern)
Balchen, Steen (Intern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD


Department of Chemical and Biochemical Engineering
Period: 15/07/2007 → 29/09/2010
Number of participants: 6
PhD Student:
Conte, Elisa (Intern)
Supervisor:
Abildskov, Jens (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Skov, Anne Ladegaard (Intern)
Jiménez-González, Concepción (Ekstern)
Kate, Antoon J. B. ten (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Integration of Modelling, Design and Control for Efficient Operation of chemical Processes
Department of Chemical and Biochemical Engineering
Period: 01/07/2007 → 13/04/2011
Number of participants: 6
Phd Student:
Abd Hamid, Mohd Kamaruddin Bin (Intern)
Supervisor:
Sin, Gürkan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Manan, Zainuddin Abdul (Ekstern)
Skogestad, Sigurd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Process-Product Synthesis, Design and Analysis through the Group-Contribution Approach
Department of Chemical and Biochemical Engineering
Period: 01/04/2007 → 01/09/2010
Number of participants: 7
Phd Student:
Alvarado-Morales, Merlin (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Woodley, John (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Camarda, Kyle V. (Ekstern)
Zondervan, Edwin (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Model-Based Computer Aided Framework for Design of Process Monitoring and Analysis Systems
Department of Chemical and Biochemical Engineering
Number of participants: 6
Phd Student:
Singh, Ravendra (Intern)
Supervisor:
Gernaey, Krist V. (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Woodley, John (Intern)
Venkatasubramanian, Venkat (Ekstern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Molecular Design using Grid Technology
Department of Chemical and Biochemical Engineering
Period: 01/06/2006 → 23/09/2009
Number of participants: 6
Phd Student:
Chelakara Satyanarayana, Kavitha (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Abildskov, Jens (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Adjiman, Claire S. (Ekstern)
Camarda, Kyle V. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Computer-Aided Multiscale Modelling for Chemical Product-Process Design
Department of Chemical and Biochemical Engineering
Period: 01/02/2006 → 26/08/2009
Number of participants: 5
Phd Student:
Morales Rodriguez, Ricardo (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Cisneros, Eduardo Salvador P. (Intern)
Harper, Peter Mathias (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Model-Based Retrofit Design and Analysis of Petrochemical Processes
Department of Chemical and Biochemical Engineering
Period: 01/01/2006 → 04/11/2009
Number of participants: 5
Phd Student:
Rashed, Jamal Elbashir Ali (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Clement, Karsten (Intern)
Eden, Mario Richard (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Development of Group Contribution plus Models for Properties of Organic Chemical Systems
Department of Chemical and Biochemical Engineering
Period: 01/10/2005 → 26/08/2009
Number of participants: 6
Phd Student:
Gonzalez Villalba, Hugo Edson (Intern)
Supervisor:
Abildskov, Jens (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Cisneros, Eduardo Salvador P. (Intern)
Schiller, Martin (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Modelling and Design of Chemically Formulated Products
Department of Chemical and Biochemical Engineering
Period: 01/11/2004 → 26/06/2008
Number of participants: 7
Phd Student:
Soni, Vipasha (Intern)
Supervisor:
Abildskov, Jens (Intern)
Jonsson, Gunnar Eigil (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Drioli, Enrico (Ekstern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Computer Aided Modelling for Bio- and Chemical, Process/Product Design
Department of Chemical and Biochemical Engineering
Period: 01/12/2002 → 30/05/2006
Number of participants: 5
Phd Student:
Sales Cruz, Alfonso Mauricio (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Cisneros, Eduardo Salvador P. (Intern)
**Integrated Process/Product Synthesis and Design Through a Reverse Modelling Approach**

Department of Chemical and Biochemical Engineering  
Period: 01/09/2002 → 07/03/2006  
Number of participants: 5  
Phd Student:  
d'Anterroches, Loïc (Intern)  
Main Supervisor:  
Gani, Rafiqul (Intern)  
Examiner:  
Villadsen, John (Intern)  
Kraslawski, Andrzej (Ekstern)  
Pistikopoulos, Stratos (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Modeling, Design, Operability and Analysis of Reaction-Separation Systems**

Department of Chemical and Biochemical Engineering  
Period: 01/09/2002 → 07/03/2006  
Number of participants: 5  
Phd Student:  
Ramirez Jimenez, Edgar (Intern)  
Main Supervisor:  
Gani, Rafiqul (Intern)  
Examiner:  
Jørgensen, Sten Bay (Intern)  
Górak, Andrzej (Ekstern)  
Perregaard, Jens (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Anden EU-finansiering  
Project: PhD

**Modelling of Pesticide Properties in Polymers and Pesticide Uptake in Plants Leafs**

Department of Chemical and Biochemical Engineering  
Period: 01/08/2002 → 07/03/2006  
Number of participants: 5  
Phd Student:  
Muro Sunè, Nuria (Intern)  
Main Supervisor:  
Gani, Rafiqul (Intern)  
Examiner:  
Abildskov, Jens (Intern)  
Harper, Peter Mathias (Intern)  
Heming, Alexander Mark (Ekstern)

**Financing sources**
Modelling, Simulation and Optimization of Anaerobic Biogas Processes

Department of Chemical and Biochemical Engineering
Period: 01/03/2002 → 30/04/2002
Number of participants: 2
Phd Student:
Velusami, Balasubramanian (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

Modelling for Predictive Control

Department of Chemical and Biochemical Engineering
Period: 01/11/2001 → 22/01/2007
Number of participants: 6
Phd Student:
Li, Hongwen (Ekstern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Abildskov, Jens (Intern)
Andersen, Henrik Weisberg (Ekstern)
Jacobsen, Elling W. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering
Project: PhD

Integration of synthesis, design and control of batch operations for product design

Department of Chemical and Biochemical Engineering
Period: 01/06/2000 → 07/03/2006
Number of participants: 5
Phd Student:
Papaoikonomou, Eirini (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Abildskov, Jens (Intern)
Morrison, James William (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden sektorministeriel finans
Project: PhD
Thermodynamic insights based integration of process synthesis, design and control

Department of Chemical and Biochemical Engineering
Period: 01/10/1999 → 28/02/2003
Number of participants: 5
PhD Student:
Bek-Pedersen, Erik (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Górak, Andrzej (Ekstern)
Sørensen, Esben Lauge (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: DTU-lænnet stipendie
Project: PhD

Alternative metoder til energieffektive stofadskillelser

Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 21/12/2003
Number of participants: 6
PhD Student:
Eden, Mario Richard (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Kiil, Søren (Intern)
Cordiner, Joan (Ekstern)
Kraslawski, Andrzej (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt CAMP
Project: PhD

Global CAPE-OPEN
EU-Funded project

Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 31/12/2001
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

Financial sources
Source: Unknown
Name of research programme: Uendt
Amount: 1,000,000.00 Danish Kroner
Project

Optimisation Techniques for Process Synthesis, Design and control

Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 31/03/2001
Number of participants: 2
PhD Student:
Henriksen, Jens Peter (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt EU-finansieret
Project: PhD

Computer Aided Process/Phenomena Modelling Based on Data
Department of Chemical and Biochemical Engineering
Period: 01/02/1999 → 15/03/2001
Number of participants: 2
Phd Student:
Nielsen, Thomas Lund (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

HYSEP
EU-Funded project
Department of Chemical and Biochemical Engineering
Period: 01/02/1998 → 01/02/2001
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 800,000.00 Danish Kroner
Project

Integrated Simulation System with thermodynamic insight
Department of Chemical and Biochemical Engineering
Period: 01/02/1998 → 01/11/2000
Number of participants: 3
Phd Student:
Russel, Boris Mariboe (Intern)
Supervisor:
Jørgensen, Sten Bay (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Project: PhD

Integrated approach to computer aided process synthesis
Department of Chemical and Biochemical Engineering
Period: 01/10/1997 → 20/09/2002
Number of participants: 5
Phd Student:
Hostrup, Martin (Intern)
A.1 Activity coefficient models
The objective of this project is to develop new models that will enhance the application range of group contribution approaches. Currently, we have two active projects in this area. The first is a PhD-level project whose objective is to develop a second-order model for estimation of liquid phase activity coefficients considering UNIFAC as the basic (first-order) model. The principal idea is that through the addition of a second-order term, some of the well-known limitations of the UNIFAC model can be overcome. Since the UNIFAC (first-order) groups are limited in terms of the molecular structural information they can provide, they are also limited to the contributions they can provide to the corresponding activity coefficient value of the molecule in a liquid mixture with other molecules. The second-order term, which is added to the original first order expression, has been derived through Taylor series expansion of the first-order model with respect to the group interaction parameters (second-order). The second project in this section deals with the development of a software library containing a large collection of activity coefficient models that can be used for various applications (in-house or external). Activity coefficient models suitable for mixtures with electrolyte systems are also being studied.

A.2 Pure component property estimation methods and software
In the area of pure component property estimation methods, we have concentrated our efforts on the development of new methods for properties not covered by us before, and, in the extension of existing methods to also cover compounds with complex molecular structures (heterocyclic-ring, multi-ring, and large molecules). The properties have been classified as primary (can be estimated only from molecular structural information), secondary (can be estimated from other known properties) and functional (depends on temperature, pressure and/or composition). New methods have been developed mainly for primary properties. For secondary properties, well known and well tested correlations have been programmed and included in the property prediction software (ProPred). For functional properties, two options have been developed. In
the first option, given the data and a function, the function parameters are determined through regression. In the second option, data are generated through an equation of state or corresponding states model and then fitted to a specified function. In the primary property estimation area, the melting point method of Constantinou and Gani is being revised and a new model for estimation of the standard heats of fusion is being developed. For primary properties, the Constantinou & Gani method as well as the Joback method has been added in ProPred. The primary property estimation methods are also being extended to polymers. In the secondary property area, a large collection of methods has been tested and added to ProPred (properties such as solubility parameter, refractive index, and many more have been added). A new atom contribution method (proposed by Wilson) is being currently added to ProPred. In the functional property area, generation and regression of temperature dependent data for vapour pressures is now possible. Other properties to be included soon are surface tension, viscosity, density, thermal conductivity and heat capacity.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Harper, Peter Mathias (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

A.3 Computation of chemical and/or physical equilibrium
Computation of phase equilibrium (with or without chemical reaction) continues to be an important part of our research effort. This is because in our opinion, phase diagram based design/analysis provide a simple yet accurate way of visualising the operation of processes where phase equilibrium has a significant role. A major effort has been devoted to the computation of simultaneous chemical and physical equilibrium based on a new algorithm (PhD-thesis of Eduardo Perez-Cisneros, 1997). Employing an element-approach, the new algorithm reduces the dimension of the problem, thereby, providing the visualisation of the phase behaviour for multi-component systems in two- or three-dimensional phase diagrams. The new algorithm is also able to compute the presence of "element" reactive azeotropes. A unique feature of the new algorithm is that, the computation of the element-based chemical and physical equilibrium problem is identical to that of computation of component based physical equilibrium problem. CAPEC has earlier developed a collection of robust and efficient physical equilibrium computational modules (such as location of binary azeotropes, SLE and high pressure VLE). In the area of electrolytes, CAPEC has started a new PhD-level project where issues related to prediction of activity coefficients for calculation of PH and solubility diagrams for mixtures with electrolyte systems are being addressed. Known activity coefficients are being examined for their applicability and the unavailable model parameters are being estimated through a developed parameter estimation program. Since data for many electrolyte systems are limited to a few measured points, a thorough analysis of the sensitivity of the activity coefficient model parameters is being made. Preliminary results from the sensitivity analysis show that not all the model parameters need to be estimated as only a few affects the activity coefficient value.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 4
Project participant:
Jensen, Anne Krogh (Intern)
Takano, Kiyoteru (Intern)
Hostrup, Martin (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

A.4 Data visualisation and parameter estimation
A computer aided system targeted on the identification of relationships between compound structure/class and properties, maintenance of a validated sets of experimental data and assisting in the development of new group contribution methods is under development. The software, called DATA, is currently able to: Show single component properties, and allow the user to add data to an existing database or to create a new database. Show properties for a subset of compounds (chosen by the user), with tabular presentation and with graphical presentation. Show mixture properties (tabular presentation and graphical presentation). Currently, the available mixture properties are infinite dilution activity coefficients and VLE-data. A small database, containing carefully screened and selected experimental data, is part of the DATA software. Since all model development activities require parameter estimation, another project in this section deals with the development of general parameter estimation software that will be used in all model development work. The future plans in this area is to add more properties (pure component and mixture) and integrate DATA to a parameter estimation program so that new property estimation method can be developed as well as existing model parameters can be re-estimated with new data or with selected sub-sets of data.
A.5 Databank management and access tools
Access to data and parameters of various kinds, is of key importance in order to perform almost any task in CAPE. In order to ease the task of database maintenance and improve access times, storage and retrieval of data, it is desirable to use advanced database features and formats. The goal is to develop one single structure capable of fulfilling the data needs of all programs developed within CAPEC and for use within ICAS (see program research E and CAPEC software). A study of the needs and demands of the various programs within CAPEC has been started and minor tests of database engines and access tool have been performed. Current and future plans include the formalisation of the database/databank structure and the development of the needed routine library for data access and maintenance.

A. Correlation/prediction of thermo-physical and phase equilibrium properties
Similar synthesis (flowsheet generation) algorithms are also being developed for pharmaceutical and biochemical processes. Since, compared to the chemical processes, these processes are considerably different, the synthesis algorithm needs modifications. This is primarily because many of the needed properties may not be available. Therefore, new definitions of relationships between separation techniques and process design independent of the properties need to be developed. It has been possible to graphically generate feasible process flowsheets together with the corresponding conditions of operation through the use of solubility diagrams of mixtures with electrolyte systems. These methods are now being converted into computer aided synthesis and design techniques. Research on hybrid separation processes has been started. The principle of hybridisation has been defined as the use of two or more separation techniques at their highest separation efficiencies in order to perform a desirable separation. As an example, consider the separation of aqueous azeotropic mixtures. By conventional distillation alone it is not possible to obtain pure products because of the azeotrope. However, for those azeotropes that are at the low concentration range of water, pervaporation is highly efficient to remove the last amounts of water (starting at the azeotropic point and ending at the pure product). The objective of the project is to develop computer aided synthesis and design techniques for generation of hybrid separation schemes that are energy efficient and environmentally benign. This project is funded by the European Union and has partners from UK, Belgium and Greece.
C.2 Computer Aided Molecular Design (CAMD)
Computer aided molecular design (CAMD) provides a means for determining molecules having a desirable set of physico-chemical properties. As the physico-chemical properties are directly or indirectly related to the structure of the molecule(s), methodologies for CAMD are typically based on "exploiting" these relationships. A multi-level approach is currently under development. In this approach each level has its own generation and testing steps. The results from each level "trickle down" to the next level. This ensures that the size of the combinatorial problem is continuously held at a level where it can be handled effectively without any so-called "combinatorial explosion". Furthermore, by having the most time consuming operations at the higher levels where the remaining candidates are the most promising, efficiency with respect to execution time is naturally obtained. Since the actual calculation/estimation of the properties is done using purely predictive methods, the accuracy, speed and applicability (with respect to level of detail needed in the molecule description) are aspects which have to be taken into considerations when selecting how and where to apply the various methods. Note that there may be several different available methods. It is possible to design molecules with a significant level of detail (down to a 3-dimensional model on atomic level) without suffering from combinatorial explosion and without sacrifice of computational accuracy. Once a 3-dimensional model is obtained results can be exported directly into molecular modelling programs for further analysis. Current work is also investigating the developing of an interactive CAMD feature. The objective here is to design the molecule with desirable properties through interaction with the user.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → ...
Number of participants: 2
Project participant:
Harper, Peter Mathias (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

C.3 Design and analysis
Aspects of design and analysis of separation processes such as azeotropic distillation, reactive distillation, membrane-based gas separation, crystallisation have been investigated. Also, the design and analysis of various types of reactor operations have been investigated. Operation of azeotropic distillation and fixed bed reactors were studied in detail. In the case of reactive distillation, the element-based approach used for modelling these processes permitted the development of a suite of simple graphical design/analysis techniques. A unique feature of these techniques is that an element-based reactive distillation is identical to component-based non-reactive distillation. Therefore, by incorporating the element transformations on the well known component-based non-reactive distillation design techniques (such as the McCabe-Thiele method, the residue curves, distillation boundaries, the Lewis-Matheson method, etc.), it has been possible to employ these techniques also for design of reactive distillation. In the membrane-based separation processes, use of orthogonal collocation method permitted the simultaneous computation of analytical sensitivities, that is, derivatives of the model output variables with respect to any parameter in the equation system. This resulted in an efficient and versatile module that can be used for simulation and design as well as for optimisation and parameter estimation calculations.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → ...
Number of participants: 8
Project participant:
Recke, Bodil (Intern)
Andersen, Torben Ravn (Intern)
Hostrup, Martin (Intern)
Takano, Kiyoteru (Intern)
Tessendorf, Stefan (Intern)
Lei, Frede (Intern)
Pedersen, Kurt (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)

C. Process synthesis, process/product design and analysis
Three areas of research have received attention during the last twelve months. The objective of the first project is the development of a generalised methodology for generation of physically feasible process flowsheets. The thermodynamic insights based synthesis method developed earlier by Jaksland (PhD thesis Cecilia Jaksland, 1996) is further developed
to include new definitions of properties-separation process relationships, to include new properties and separation processes and to include rules which enable the application of the synthesis algorithm when properties are not available. Also, the new algorithm can include the reactor in the flowsheet. The methodology employs a four-step procedure: a) mixture analysis, b) calculation of component property ratios, c) using the results of the previous steps to find the feasible separation techniques and d) listing the possible alternatives of the feasible separation techniques.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → ...
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

E.1 Process Integration
A project concerning development of a simulation tool (steady state as well as dynamic) for Petlyuk distillation columns has been initiated. The objective for development of this tool is to study the operation of integrated distillation trains. Distillation column configuration for the separation of azeotropic mixtures continues to attract industrial and academic researchers. For heterogeneous azeotropic mixture separation, the advantages and disadvantages of the "direct-sequence" and the "indirect-sequence" have been studied at CAPEC. The conditions, under which the undesirable effects of multiple solutions can be avoided, have been identified for various design/operational alternatives.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → ...
Number of participants: 3
Project participant:
Andersen, Torben Ravn (Intern)
Jørgensen, Sten Bay (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

E.2 System (Tools) Integration
ICAS: Intergrated Computer Aided System Solutions of process integration problems require an integrated set of tools. There is a demand for tools that will enable the engineer to directly transfer information between various phases of process design, process analysis, and process optimisation. Therefore, an integrated computer aided system for process modelling, simulation, design, synthesis and analysis has been developed. This system includes a simulation (steady state and dynamic) engine and tools for physical properties estimation, process/product synthesis and process/product design. The total system, called ICAS, has been evaluated against various test problems. A major part of the tools integration within ICAS has been developed through a PhD-project (PhD thesis of Anne K. Jensen, May 1998), where, emphasis has also been given to the development of a computer aided modelling system. The model generation feature in ICAS consists of a generic modelling language for interactive definition of new building objects and a knowledge-based modelling language that apply rules in order to create new building objects. The methodology for creation of building objects is essentially based on information related to definition of control shells (boundary, physical description of the interior, and interactions between the shell and the surrounding). From the definition of the control shell, the computer aided modelling system generates the model equations describing the control shell. In addition to the creation of new objects, a system for graphical aggregation of the building object into a composite model has also been developed. Finally, integration of the model generator to a process simulator allows direct simulation with the generated model (the appropriate code for the simulator is generated by the model generation feature).

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → ...
Number of participants: 7
Project participant:
Jensen, Anne Krogh (Intern)
Russel, Boris Mariboe (Intern)
Harper, Peter Mathias (Intern)
Hostrup, Martin (Intern)
Jørgensen, John Bagterp (Intern)
Andersen, Torben Ravn (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project
E.3 Integrated Algorithms
Integration of process synthesis, design and control In design of continuous process flowsheets, it is desirable to limit the variety of possible flowsheets as early as possible. If screening of flowsheets is done entirely on the basis of steady state economics, it will often lead to solutions where dynamic behaviour causes the final plant to be difficult to control (or even impossible to control). It is therefore desirable to have an integrated set of tools through which design and control engineers can find feasible flowsheets from steady state information alone, at an early stage of the project. The plan for this project is to develop an integrated approach to design, synthesis and control of chemical processes on the basis of thermodynamic insights. The goal is to present a methodology which leads to a flowsheet of a process where aspects of design (condition of operation), synthesis (choice of unit operations) and operability (energy requirements, controllability, environmental impact, etc.) are addressed in an integrated manner. This methodology will be applicable to design of new processes or for determining appropriate alternatives for existing processes (retrofit problems). Inclusion of all sub problems into the objective of the design (for the optimal solution) will provide a multi parametric function. The trade off between the various terms will be analyzed through "trade off curves". Thermodynamic insights will help to understand these curves and to apply them in the integrated approach.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 3
Project participant:
Lewin, D.R. (Ekstern)
O’Connell, J.P. (Ekstern)
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

E. Process and Tools Integration
Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

F.1 Numerical Methods Collection
Optimisation techniques DAE-solvers. The objective of this project is collect and implement numerical methods suitable for inclusion into the solver toolbox of ICAS. ICAS requires numerical routines for algebraic equations solving, differential and algebraic equation solving, partial differential equation (plus algebraic equations) solving, optimisation methods and many more. A project to implement, update and validate optimisation methods and DAE-solvers has been started. NLP as well as MINLP methods are being implemented under optimisation techniques. Index-one DAE-solvers (with initialisation feature) with options for switching between stiff/non-stiff methods, dense/sparse methods and DAE/ODE modes of simulation are being investigated.

Department of Chemical and Biochemical Engineering
Period: 01/05/1997 → …
Number of participants: 2
Project participant:
Jensen, Anne Krogh (Intern)
Project Manager, organisational:
Gani, Rafiqul (Intern)
Project

F.2 Initialisation for large problems
Distillation simulation Solution of very large steady state simulation problems (more than 10000 equations and variables) may require very long computing times, even with the fastest computers. If steady state simulation is performed for process optimisation, even longer computing times may be necessary. One way of reducing the computing times is to provide better initial estimates so that a faster convergence to the solution can be obtained for the simulation/optimisation problem. For single and multiple column distillation problems, an efficient initialisation procedure has been developed and validated with several test examples. Large reduction of computational times have been achieved by first solving a reduced problem. A unique feature of the reduced problem is that it represents a linear set of algebraic equations and the key distillation model variables (for the large problem) is predicted with reasonable accuracy, thereby, providing very good initial estimates. The applicability of this approach for other problems will be investigated in future.
F.3 Simulation strategy
Flow sheet decomposition and equation ordering. Solution of flowsheet simulation problems with the modular approach requires flowsheet decomposition techniques so that the appropriate calculation order can be specified to the solver. The same problem when solved with the equation oriented approach, needs the equations to be ordered (if possible) in a particular manner so that the solution efficiency can be improved. In an integrated approach to process simulation, design and control, the simulation engine needs to be flexible so that it is possible to move from one mode of simulation to another without much extra work. Also, if simulation engine is provided from two different sources employing two different solution approaches, they may need to interact through a common set of variables. It may also be that in the same process flowsheet, one part is suitable for solution with the modular approach while another part may be suitable for the equation oriented approach. The same may be true for dynamic simulation of a process flowsheet containing dynamic and non-dynamic units. The objective of this project is to determine appropriate simulation strategies for the simulation engine so that mixed mode (steady state/dynamic, equation oriented/modular, ODE/DAE) simulation is possible with increased solution efficiency and robustness. Since all simulation problems need the same flowsheet topology information, this information may also be used to link flowsheet decomposition and equation ordering. ICAS (see program E) has a built-in feature for defining any problem specific simulation strategy. Current and future work will take these ideas further with a view to the development of generalized strategies of wide application range.

A Multi-phase, Multi-level Framework for Computer aided Molecular Design
Department of Chemical and Biochemical Engineering
Period: 01/02/1997 → 25/07/2000
Number of participants: 4
Phd Student:
Harper, Peter Mathias (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Ekperiment
Project: PhD
Optimal design og operation af procesintegreret destillation
Department of Chemical and Biochemical Engineering
Period: 01/02/1997 → 24/01/2003
Number of participants: 5
Phd Student:
Andersen, Torben Ravn (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Gani, Rafiqul (Intern)
Andersen, Henrik Weisberg (Ekstern)
Skogestad, Sigurd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

Computer Aided Modelling
Department of Chemical and Biochemical Engineering
Period: 01/09/1995 → …
Number of participants: 1
Project Manager, organisational:
Gani, Rafiqul (Intern)

Generel Model til gruppebidragsbaseret forudsigelse af faseligevægte af komplekse blandinger
Department of Chemical and Biochemical Engineering
Period: 01/09/1995 → …
Number of participants: 3
Phd Student:
Abildskov, Jens (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Elbro, Helle Simon (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Modeling, Analyses and Design of
Department of Chemical and Biochemical Engineering
Period: 01/09/1995 → 19/07/1999
Number of participants: 4
Phd Student:
Tessendorf, Stefan (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Cameron, David (Ekstern)
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD
Modelling, Design and Analysis of Complex Separation Processes

Department of Chemical and Biochemical Engineering
Number of participants: 4
Phd Student:
Cisneros, Eduardo Salvador P. (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Christiansen, Lars J. (Ekstern)
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden International Finan-SU
Project: PhD

Design and Simulation of Integrated Biochemical Processes

Department of Chemical and Biochemical Engineering
Period: 01/09/1994 → 20/10/1999
Number of participants: 3
Phd Student:
Bagherpour, Khosrow (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Wiebe, Lars (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Development of a computer aided system for process simulation model generation

Department of Chemical and Biochemical Engineering
Period: 01/08/1994 → 02/08/1999
Number of participants: 4
Phd Student:
Jensen, Anne Krogh (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Jørgensen, Sten Bay (Intern)
Sørensen, Esben Lauge (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Separation process synthesis, design and analysis based on thermodynamic insights.

Department of Chemical and Biochemical Engineering
Period: 01/10/1992 → 23/04/1996
Number of participants: 2
Phd Student:
Jaksland, Cecilia (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Nordisk finansiering
Project: PhD

Design og analyse af superkritiske ekstraktionsprocesser.
Department of Chemical and Biochemical Engineering
Period: 01/06/1992 → 18/12/1995
Number of participants: 2
Phd Student:
Hytoft, Glen (Intern)
Main Supervisor:
Gani, Rafiqul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådene via projektbe
Project: PhD

Simulering og optimering af ammoniakanlæg
Department of Chemical and Biochemical Engineering
Period: 01/04/1991 → ...
Number of participants: 5
Phd Student:
Bossen, Bjarne Skak (Intern)
Supervisor:
Christiansen, Lars J. (Ekstern)
Main Supervisor:
Gani, Rafiqul (Intern)
Examiner:
Gravesen, Peter (Ekstern)
Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ATV- Gammel ordning
Project: PhD

Activities:

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

Description

Related event
Asset management for enhancing energy efficiency in water and wastewater systems
24/04/2013 → 26/04/2013
Marbella, Spain
Selection and design of solvents
Period: 21 Apr 2013 → 24 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description
Oral conference presentation: Rafiqul Gani, 2013, "Selection and design of solvents", Plenary Lecture

Related event
23rd Croatian Meeting of Chemists and Chemical Engineers
21/04/2013 → 24/04/2013
Osijek, Croatia
Activity: Talks and presentations › Conference presentations

Computer-aided modeling framework: a generic template as a modeling tool
Period: 20 Apr 2013 → 25 Apr 2013
Rafiqul Gani (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Description

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology
Period: 20 Apr 2013 → 25 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Center for Energy Resources Engineering
CERE – Center for Energy Resources Engineering

Description
Oral conference presentation: Michele Mattei, Peter Krogh, Bo Depner, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, "Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology"

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Efficient Information and Data Management in Synthesis and Design of Processing Networks
Period: 20 Apr 2013 → 25 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description
Oral Conference Presentation: A. Quaglia, G. Sin, R. Gani, 2013, "Efficient Information and Data Management in Synthesis and Design of Processing Networks"

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel
Period: 20 Apr 2013 → 25 Apr 2013
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description
Oral Conference Presentation: Larissa P. Cunico, Roberta Ceriani, Bent Sarup, Rafiqul Gani, 2013, "Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel"

Related event
9th European Congress of Chemical Engineering
21/04/2013 → 25/04/2013
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

Recent advances in CAPE and PSE applicable to the Pharmaceuticals Industry
Period: 19 Dec 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description
AstraZeneca, UK

Related external organisation

Computational Solvent Design for Integrated Chemical Processes
Period: 15 Nov 2012 → 16 Nov 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Pesticide uptake modeling
Period: 7 Nov 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description
Rafiqul Gani, 2012, “Pesticide uptake modeling”, Syngenta, Jealott’s International Research Centre, UK, 7 November
Related external organisation

Research at CAPEC
Period: 27 Sep 2012
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description
Rafiqul Gani, 2012, “Research at CAPEC”, Mitsubishi Research Center, Mizushima, Japan, 27 September
Related external organisation

Building and sustaining an Industrial Consortium – The experience of DTU-CAPEC
Period: 22 Apr 2011
Rafiqul Gani (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Related event
Building and sustaining an Industrial Consortium – The experience of DTU-CAPEC: UTM, Johor Bahru, Malaysia, 22 April
22/04/2011 → 22/04/2011
Johor Bahru, Malaysia
Activity: Talks and presentations › Conference presentations

Managing the Complexity in Product and Process Engineering
Period: 17 Mar 2011
Rafiqul Gani (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Description
Departmental Seminar
Related external organisation
National Technical University of Athens
Greece
CAPEC Overview and Status - 2011
Period: 10 Feb 2011
Rafiqul Gani (Speaker)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center

Related event
CAPEC Overview and Status - 2011: Invited Seminar
10/02/2011 → …
Lonza, Switzerland
Activity: Talks and presentations › Conference presentations

CAPEC Overview and Status - 2011
Period: 27 Jan 2011
Rafiqul Gani (Invited speaker)
Computer Aided Process Engineering Center
Department of Chemical and Biochemical Engineering

Related external organisation
DSM
Netherlands
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations