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1. CFD simulation of transient stage of continuous countercurrent hydrolysis of canola oil
   10 August 2012
   Wei-Cheng Wang | Robert H. Natelson | Larry F. Stikeleather | William L. Roberts

   **Abstract:** Computational Fluid Dynamic (CFD) modeling of a continuous countercurrent hydrolysis process was performed using ANSYS-CFX. The liquid properties and flow behavior such as density, specific heats, dynamic viscosity, thermal conductivity, and thermal expansivity as well as water solubility of the hydrolysis components triglyceride, diglyceride, monoglyceride, free fatty acid, and glycerol were calculated. Chemical kinetics for the hydrolysis reactions were simulated in this model by applying Arrhenius parameters. The simulation was based on actual experimental reaction conditions including temperature and water-to-oil ratio. The results not only have good agreement with experimental data but also show instantaneous distributions of concentrations of every component in hydrolysis reaction. This model provided visible insight into the continuous countercurrent hydrolysis process.

2. Model predictive control: past, present and future
   1 May 1999
   Manfred Morari | Jay H. Lee

   **Abstract:** More than 15 years after model predictive control (MPC) appeared in industry as an effective means to deal with multivariable constrained control problems, a theoretical basis for this technique has started to emerge. The issues of feasibility of the on-line optimization, stability and performance are largely understood for systems described by linear models. Much progress has been made on these issues for non-linear systems but for practical applications many questions remain, including the reliability and efficiency of the on-line computation scheme. To deal with model uncertainty ‘rigorously’ an involved dynamic programming problem must be solved. The approximation techniques proposed for this purpose are largely at a conceptual stage. Among the broader research needs the following areas are identified: multivariable system identification, performance monitoring and diagnostics, non-linear state estimation, and batch system control. Many practical problems like control objective prioritization and symptom-aided diagnosis can be integrated systematically and effectively into the MPC framework by expanding the problem formulation to include integer variables yielding a mixed-integer quadratic or linear program. Efficient techniques for solving these problems are becoming available.

3. Sustainable design and synthesis of hydrocarbon biorefinery via gasification pathway: Integrated life cycle assessment and technoeconomic analysis with multiobjective superstructure optimization
   10 May 2013
   Belinda Wang | Berhane H. Gebreslassie | Fengqi You

   **Abstract:** This paper proposes a multiobjective, mixed-integer nonlinear programming (MINLP) model for the superstructure optimization of hydrocarbon biorefineries via gasification pathway under economic and environmental criteria. The proposed hydrocarbon biorefinery superstructure includes a number of major processing stages, such as drying of the cellulosic biomass feedstocks, air separation unit, gasification, syngas conditioning, Fischer–Tropsch synthesis, hydroprocessing, power generation, and the diesel and gasoline production. The superstructure considers alternatives of technologies and equipment, such as gasification technologies, cooling options, hydrogen production sources, and Fischer–Tropsch synthesis catalysts. The economic objective is measured by the net present value (NPV), and the environmental concern is measured using global warming potential (GWP) that follows the life cycle assessment procedures, which evaluates the gate-to-gate environmental impacts of hydrocarbon biofuels. The multiobjective MINLP model simultaneously determines the technology selection, operation conditions, flow rate of each stream, energy consumption of each unit, economic performance, environmental impacts, and equipment sizes. The multiobjective MINLP problem is solved with the ε-constraint method. The resulting Pareto-optimal curve reveals the trade-off between the economic and environmental performances. The optimal solution reveals...
that the high-temperature gasification, direct cooling, internal hydrogen production and cobalt catalysis have
the best environmental and economic performances. At the breakeven point, where the optimal NPV is 0, the
unit production cost of hydrocarbon biorefinery is $4.43 per gasoline-equivalent gallon (GEG) with unit GWP of
20.92kg CO2 eqv./GEG. In the case of maximum NPV of $810 MM, the corresponding unit production cost is
$3.17/GEG.

4. Process synthesis of hybrid coal, biomass, and natural gas to liquids via Fischer–Tropsch
synthesis, ZSM-5 catalytic conversion, methanol synthesis, methanol-to-gasoline, and methanol-
to-olefins/distillate technologies

20 December 2012
Richard C. Baliban | Josephine A. Elia | Vern Weekman | Christodoulos A. Floudas

Abstract: Several technologies for synthesis gas (syngas) refining are introduced into a thermochemical based
superstructure that will convert biomass, coal, and natural gas to liquid transportation fuels using Fischer–
Tropsch (FT) synthesis or methanol synthesis. The FT effluent can be (i) refined into gasoline, diesel, and
kerosene or (ii) catalytically converted to methanol and distillate over a ZSM-5 zeolite. Methanol can be
converted using ZSM-5 (i) directly to gasoline or to (ii) distillate via olefin intermediates. A mixed-integer
nonlinear optimization model that includes simultaneous heat, power, and water integration is solved to global
optimality to determine the process topologies that will produce the liquid fuels at the lowest cost. Twenty-four
case studies consisting of different (a) liquid fuel combinations, (b) refinery capacities, and (c) superstructure
possibilities are analyzed to identify important process topological differences and their effect on the overall
system cost, the process material/energy balances, and the well-to-wheel greenhouse gas emissions.

5. Life cycle optimization for sustainable design and operations of hydrocarbon biorefinery via fast
pyrolysis, hydrotreating and hydrocracking

5 March 2013
Berhane H. Gebreslassie | Maxim Slivinsky | Belinda Wang | Fengqi You

Abstract: This paper addresses the optimal design and operation of hydrocarbon biorefinery via fast pyrolysis,
ychodotreating and hydrocracking of hybrid poplar feedstock under economic and environmental criteria. The
hydrocarbon biorefinery encompasses fast pyrolysis for crude bio-oil production, upgrading of the bio-oil
through hydrotreating, separation and hydrocracking of long chained hydrocarbons into gasoline and diesel
range products, and steam reforming for hydrogen production. We propose a bi-criteria nonlinear
programming (NLP) model that seeks to maximize the economic performance measured by the net present
value (NPV) and to minimize the environmental impacts. The environmental objective is measured with the
global warming potential (GWP) metric according to the life cycle assessment procedures, which covers
gate-to-gate environmental impacts of the hydrocarbon biorefinery. The multiojective NLP model
simultaneously determines the production capacity, size of each process units, operational conditions, the flow
rates of species and streams at each stage of the process, hydrocarbon biofuel yields, and consumption rate
of feedstock, steam, electricity, and natural gas. The bi-criteria NLP model is solved with the ε-constraint
method, and the resulting Pareto-optimal curve reveals the trade-off between the economic and environmental
dimensions of the sustainable hydrocarbon biorefinery. The optimization results reveal that the unit production
cost of the hydrocarbon biofuels is $2.31 per gallon of gasoline equivalent (GGE) for the maximum NPV
solution and $3.67/GGE for the minimum GWP design. The corresponding greenhouse emission is
8.07kgCO2-eq/GGE.


15 March 2003
Venkat Venkatasubramanian | Raghunathan Rengaswamy | Surya N. Kavuri | Kewen Yin

Abstract: In this final part, we discuss fault diagnosis methods that are based on historic process knowledge.
We also compare and evaluate the various methodologies reviewed in this series in terms of the set of
desirable characteristics we proposed in Part I. This comparative study reveals the relative strengths and
weaknesses of the different approaches. One realizes that no single method has all the desirable features one
would like a diagnostic system to possess. It is our view that some of these methods can complement one
another resulting in better diagnostic systems. Integrating these complementary features is one way to
develop hybrid systems that could overcome the limitations of individual solution strategies. The important role
of fault diagnosis in the broader context of process operations is also outlined. We also discuss the technical challenges in research and development that need to be addressed for the successful design and implementation of practical intelligent supervisory control systems for the process industries.

### 7. Applications of process synthesis: Moving from conventional chemical processes towards biorefinery processes

11 February 2013  
Zhihong Yuan | Bingzhen Chen | Rafiqul Gani

Abstract: 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.

### 8. Silicon solar cell production

10 August 2011  
S. Ranjan | S. Balaji | Rocco A. Panella | B. Erik Ydstie

Abstract: A significant role can be played by the systems engineering community in the optimization of the production process for silicon solar cells. Many of the techniques utilized for cell manufacturing are of recent origin and the amount of experience in the industry as a whole is limited. Some of the individual processes and steps are poorly adapted for continuous production since they were designed for micro-electronics applications rather than photovoltaics. Only very recently has the industry grown to the point where intermediate products, such as solar grade silicon, solar silicon wafers, solar cells and solar panels are commodities having global market potential. Finally, industry consolidation has generated large commercial entities which can better take advantage of tools from process systems engineering. The chemical and process systems and engineering communities can contribute to this booming industry by providing methods for improved control, process optimization and retro-fitting of existing processes, as well as encouraging process innovation and scale-up. This paper describes the complete production process for solar cells, highlights challenges relevant to systems engineering, and overviews work in three distinct areas: the application of real time optimization in silicon production, the development of scale-up models for a fluidized bed poly-silicon process and a new process concept for silicon wafer production.

### 9. Distributed model predictive control: A tutorial review and future research directions

5 April 2013  
Panagiotis D. Christofides | Riccardo Scattolini | David Muñoz de la Peña | Jinfeng Liu

Abstract: In this paper, we provide a tutorial review of recent results in the design of distributed model predictive control systems. Our goal is to not only conceptually review the results in this area but also to provide enough algorithmic details so that the advantages and disadvantages of the various approaches can become quite clear. In this sense, our hope is that this paper would complement a series of recent review papers and catalyze future research in this rapidly evolving area. We conclude discussing our viewpoint on future research directions in this area.

### 10. Supply chain optimisation for the process industries: Advances and opportunities

10 December 2009  
Lazaros G. Papageorgiou

Abstract: Supply chain management and optimisation is a critical aspect of modern enterprises and a
flourishing research area. This paper presents a critical review of methodologies for enhancing the decision-making for process industry supply chains towards the development of optimal infrastructures (assets and network) and planning. The presence of uncertainty within supply chains is discussed as an important issue for efficient capacity utilisation and robust infrastructure decisions. The incorporation of business/financial and sustainability aspects is also considered and future challenges are identified.

11. Hybrid and single feedstock energy processes for liquid transportation fuels: A critical review
11 June 2012
Christodoulos A. Floudas | Josephine A. Elia | Richard C. Baliban

Abstract: This review provides a detailed account of the key contributions within the energy communities with specific emphasis on thermochemically based hybrid energy systems for liquid transportation fuels. Specifically, the advances in the indirect liquefaction of coal to liquid (CTL), natural gas to liquid (GTL), biomass to liquid (BTL), coal and natural gas to liquid (CGTL), coal and biomass to liquid (CBTL), natural gas and biomass to liquid (BGTL), and coal, biomass, and natural gas to liquid (CBGTL) are presented. This review is the first work that provides a comprehensive description of the contributions for the single-feedstock energy systems and the hybrid feedstock energy systems, for single stand-alone processes and energy supply chain networks. The focus is on contributions in (a) conceptual design, (b) process simulation, (c) economic analysis, (d) heat integration, (e) power integration, (f) water integration, (g) process synthesis, (h) life cycle analysis, (i) sensitivity analysis, (j) uncertainty issues, and (k) supply chain. A classification of the contributions based on the products, as well as different research groups is also provided.

12. Pharmaceutical supply chains: key issues and strategies for optimisation
15 June 2004
Nilay Shah

Abstract: Supply chain optimisation is now a major research theme in process operations and management. A great deal of research has been undertaken on facility location and design, inventory and distribution planning, capacity and production planning and detailed scheduling. Only a small proportion of this work directly addresses the issues faced in the pharmaceutical sector. On the other hand, this sector is very much ready for and in need of sophisticated supply chain optimisation techniques. At the supply chain design stage, a particular problem faced by this industry is the need to balance future capacity with anticipated demands in the face of the very significant uncertainty that arises out of clinical trials and competitor activity. Efficient capacity utilisation plans and robust infrastructure investment decisions will be important as regulatory pressures increase and margins are eroded. The ability to locate nodes of the supply chain in tax havens and optimise trading and transfer price structures results in interesting degrees of freedom in the supply chain design problem. Prior even to capacity planning comes the problem of pipeline and testing planning, where the selection of products for development and the scheduling of the development tasks requires a careful management of risk and potential rewards. At the operation stage, it is often difficult to ensure responsiveness. Most pharmaceutical products involve primary active ingredient (AI) production (often multi-stage chemical synthesis or bioprocess) and secondary (formulation) production. Both of the stages are characterised by low manufacturing velocities and are hampered by the need for quality assurance activities at several points. It is not unusual for the overall supply chain cycle time to be 300 days. In this environment, supply chain debottlenecking and decoupling strategies together with co-ordinated inventory management are crucial for quick responses to changing market trends. A good understanding of what actually drives the supply chain dynamics is also required. As often as not, erratic dynamics are introduced by business processes rather than by external demand, and may be eliminated by the re-design of internal business processes or supplier/customer relationships. This paper will consider important issues in supply chain design and operation drawn from the literature and from our collaborative research projects in this area. The main features of the problems will be reviewed as will the literature to date. Some strategies for solution will be identified, as will some future research needs.

13. Integration of control theory and scheduling methods for supply chain management
5 April 2013
Kaushik Subramanian | James B. Rawlings | Christos T. Maravelias | Jesus Flores-Cerrillo | Lawrence Megan

Abstract: In this paper, we propose to use distributed model predictive control for supply chain optimization. In particular, we focus on inventory management in supply chains. We use cooperative model predictive control,
in which each agent makes their local decisions by optimizing the overall supply chain objective. Motivated by recent results in Stewart, Wright, and Rawlings (2011), we develop a new cooperative MPC algorithm that is applicable to any stabilizable system, and in particular to supply chain models. We illustrate cooperative MPC for a two node supply chain example and compare its performance and properties with other classical distributed operating policies.

14. Process systems engineering tools in the pharmaceutical industry
5 April 2013
Gregory M. Troup | Christos Georgakis

Abstract: The purpose of this paper is to provide a summary of the current state of the application of process systems engineering tools in the pharmaceutical industry. In this paper, we present the compiled results of an industrial questionnaire submitted to pharmaceutical industry professionals. The topics covered in the questionnaire include process analytics, process monitoring, plant-wide information systems, unit operation modeling, quality control, and process optimization. A futuristic view of what process systems engineering tools will enable the pharmaceutical industry will be also be presented. While the industry is regularly using the traditional Design of Experiments approach to identify key parameters and to define control spaces, these approaches result in passive control strategies that do not attempt to compensate for disturbances. Special new approaches are needed for batch processes due to their essential dependence on time-varying conditions. Lastly, we briefly describe a novel data driven modeling approach, called Design of Dynamic Experiments that enables the optimization of batch processes with respect to time-varying conditions through an example of a simulated chemical reaction process. Many more approaches of this type are needed for the calculation of the design and control spaces of the process, and the effective design of feedback systems.

15. Optimization under uncertainty: state-of-the-art and opportunities
15 June 2004
Nikolaos V. Sahinidis

Abstract: A large number of problems in production planning and scheduling, location, transportation, finance, and engineering design require that decisions be made in the presence of uncertainty. Uncertainty, for instance, governs the prices of fuels, the availability of electricity, and the demand for chemicals. A key difficulty in optimization under uncertainty is in dealing with an uncertainty space that is huge and frequently leads to very large-scale optimization models. Decision-making under uncertainty is often further complicated by the presence of integer decision variables to model logical and other discrete decisions in a multi-period or multi-stage setting. This paper reviews theory and methodology that have been developed to cope with the complexity of optimization problems under uncertainty. We discuss and contrast the classical recourse-based stochastic programming, robust stochastic programming, probabilistic (chance-constraint) programming, fuzzy programming, and stochastic dynamic programming. The advantages and shortcomings of these models are reviewed and illustrated through examples. Applications and the state-of-the-art in computations are also reviewed. Finally, we discuss several main areas for future development in this field. These include development of polynomial-time approximation schemes for multi-stage stochastic programs and the application of global optimization algorithms to two-stage and chance-constraint formulations.

16. Managing demand uncertainty in supply chain planning
15 September 2003
Anshuman Gupta | Costas D. Maranas

Abstract: In this work, we provide an overview of our previously published works on incorporating demand uncertainty in midterm planning of multisite supply chains. A stochastic programming based approach is described to model the planning process as it reacts to demand realizations unfolding over time. In the proposed bilevel-framework, the manufacturing decisions are modeled as ‘here-and-now’ decisions, which are made before demand realization. Subsequently, the logistics decisions are postponed in a ‘wait-and-see’ mode to optimize in the face of uncertainty. In addition, the trade-off between customer satisfaction level and production costs is also captured in the model. The proposed model provides an effective tool for evaluating and actively managing the exposure of an enterprises assets (such as inventory levels and profit margins) to market uncertainties. The key features of the proposed framework are highlighted through a supply chain planning case study.
17. A modular simulation package for fed-batch fermentation: penicillin production
15 November 2002
Gülnur Biroğlu | Cenk Ündey | Ali Çınar

Abstract: Simulation software based on a detailed unstructured model for penicillin production in a fed-batch fermentor has been developed. The model extends the mechanistic model of Bajpai and Reuss by adding input variables such as pH, temperature, aeration rate, agitation power, and feed flow rate of substrate and introducing the CO2 evolution term. The simulation package was then used for monitoring and fault diagnosis of a typical penicillin fermentation process. The simulator developed may be used for both research and educational purposes and is available at the web site: http://www.chee.iit.edu/~control/software.html.

18. Simulation study on biodiesel production by reactive distillation with methanol at high pressure and temperature: Impact on costs and pollutant emissions
10 May 2013
Fernando Israel Gomez-Castro | Vicente Rico-Ramirez | Juan Gabriel Segovia-Hernandez | Salvador Hernandez-Castro | Mahmoud M. El-Halwagi

Abstract: Recently, a two-step biodiesel production process which uses short-chain alcohols at supercritical conditions has been proposed. In addition, literature reports suggest that the COSMO-SAC thermodynamic model is a suitable alternative for the prediction of VLE for supercritical methanol/methyl esters mixtures. Thus, in this work a simulation study of the two-step supercritical method for the production of biodiesel is performed by using the COSMO-SAC model. Further, alternative system configurations for biodiesel production based on reactive distillation are proposed and their total emissions are compared to those corresponding to the conventional catalytic method. The study demonstrates the benefits of using reactive distillation for the esterification step and discusses the environmental impact of the supercritical production process. It has been found that the intensified alternatives reduce the emissions considerably and, through the reuse of the excess methanol, the emissions level of the supercritical process can be compared to those of the catalytic method.

19. Simulation and economic analysis of 5-hydroxymethylfurfural conversion to 2,5-furandicarboxylic acid
10 May 2013
Christoph Triebl | Vladimiros Nikolakis | Marianthi Ierapetritou

Abstract: Two processes for converting 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA) were designed using literature data together with simplified process simulation models. The main reaction step is HMF catalytic oxidation using aqueous acetic acid as solvent, Pt/ZrO2 as catalyst and air as oxidant. The first process investigated involves a mixed-suspension, mixed-product-removal crystallizer and a filter for separating solid FDCA from the solvent. The calculated minimum sale price of FDCA is $3157/t, whereas, if pure oxygen is used as oxidant the FDCA price reduces to $2458/t. Due to the high melting point of FDCA, the second alternative considered introduces trioctylamine as solvent to facilitate separation of FDCA from the solvent using distillation. The estimated FDCA price using this process is $3885/t. Sensitivity analysis shows that selectivity and conversion have small impact on FDCA price, whereas plant capacity, catalyst and HMF costs have large effects on the price of FDCA.

15 March 2003
Venkat Venkatasubramanian | Raghunathan Rengaswamy | Kewen Yin | Surya N. Kavuri

Abstract: Fault detection and diagnosis is an important problem in process engineering. It is the central component of abnormal event management (AEM) which has attracted a lot of attention recently. AEM deals with the timely detection, diagnosis and correction of abnormal conditions of faults in a process. Early detection and diagnosis of process faults while the plant is still operating in a controllable region can help avoid abnormal event progression and reduce productivity loss. Since the petrochemical industries lose an estimated 20 billion dollars every year, they have rated AEM as their number one problem that needs to be solved. Hence, there is considerable interest in this field now from industrial practitioners as well as academic researchers, as opposed to a decade or so ago. There is an abundance of literature on process fault diagnosis.
ranging from analytical methods to artificial intelligence and statistical approaches. From a modelling perspective, there are methods that require accurate process models, semi-quantitative models, or qualitative models. At the other end of the spectrum, there are methods that do not assume any form of model information and rely only on historic process data. In addition, given the process knowledge, there are different search techniques that can be applied to perform diagnosis. Such a collection of bewildering array of methodologies and alternatives often poses a difficult challenge to any aspirant who is not a specialist in these techniques. Some of these ideas seem so far apart from one another that a non-expert researcher or practitioner is often left wondering about the suitability of a method for his or her diagnostic situation. While there have been some excellent reviews in this field in the past, they often focused on a particular branch, such as analytical models, of this broad discipline. The basic aim of this three part series of papers is to provide a systematic and comparative study of various diagnostic methods from different perspectives. We broadly classify fault diagnosis methods into three general categories and review them in three parts. They are quantitative model-based methods, qualitative model-based methods, and process history-based methods. In the first part of the series, the problem of fault diagnosis is introduced and approaches based on quantitative models are reviewed. In the remaining two parts, methods based on qualitative models and process history data are reviewed. Furthermore, these disparate methods will be compared and evaluated based on a common set of criteria introduced in the first part of the series. We conclude the series with a discussion on the relationship of fault diagnosis to other process operations and on emerging trends such as hybrid blackboard-based frameworks for fault diagnosis.

21. Smart grid technologies and applications for the industrial sector
20 December 2012
Tariq Samad | Sila Kiliccote

Abstract: Smart grids have become a topic of intensive research, development, and deployment across the world over the last few years. The engagement of consumer sectors—residential, commercial, and industrial—is widely acknowledged as crucial for the projected benefits of smart grids to be realized. Although the industrial sector has traditionally been involved in managing power use with what today would be considered smart grid technologies, these applications have mostly been one-of-a-kind, requiring substantial customization. Our objective in this article is to motivate greater interest in smart grid applications in industry. We provide an overview of smart grids and of electricity use in the industrial sector. Several smart grid technologies are outlined, and automated demand response is discussed in some detail. Case studies from aluminum processing, cement manufacturing, food processing, industrial cooling, and utility plants are reviewed. Future directions in interoperable standards, advances in automated demand response, energy use optimization, and more dynamic markets are discussed.

22. A perspective on PSE in pharmaceutical process development and innovation
11 July 2012
Krist V. Gernaey | Albert E. Cervera-Padrell | John M. Woodley

Abstract: The pharmaceutical industry is under growing pressure to increase efficiency, both in production and in process development. This paper discusses the central role of Process Systems Engineering (PSE) methods and tools in pharmaceutical process development and innovation, and searches for answers to questions such as: Which PSE methods can be applied readily? Where is more method development needed? The paper covers key subjects for development of economically and environmentally sustainable pharmaceutical processes, including Process Analytical Technology in its broadest sense, continuous pharmaceutical manufacturing and green processes, and is illustrated with a series of short examples taken from the literature and ongoing research projects.

23. A complete 3D simulation of a crystallization process induced by supercritical CO2 to predict particle size
10 May 2013
Arnaud Erriguible | Tarik Fadli | Pascale Subra-Paternault

Abstract: Crystallization induced by compressed CO2 is a process that operates under several MPa of pressure. By rendering on-line measurements very difficult to perform, simulation appears as a suitable tool to better identify the important parameters of the process. A mathematical model is developed in the case of a spray-crystallization process in which a solution of minocycline-ethanol is injected into carbon dioxide as
antisolvent. The model accounts for the main physical phenomena involved, i.e. hydrodynamics, mass transfer, phase equilibrium, crystallization kinetics. Simulations are performed in 3D with a special insight in turbulence modeling. Numerical results are compared with experimental data from literature. Although experimental and simulated PSD fit satisfactorily, results emphasize the major role of the crystal–fluid interfacial tension on the accuracy. Numerical investigations are further performed to highlight the effects of injection velocity and solution concentration on the spatial distribution of the important variables in crystallization.

### 24. SustainPro—A tool for systematic process analysis, generation and evaluation of sustainable design alternatives

5 March 2013  
Ana Carvalho | Henrique A. Matos | Rafiqul Gani

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

### 25. Modelling of homogeneously catalysed reactive distillation processes in packed columns: Experimental model validation

10 January 2013  
Tobias Keller | Andrzej Górak

Abstract: The design of reactive distillation processes requires reliable and accurate models to significantly decrease the expensive and time consuming experimental work. Different modelling approaches of varying complexity are available in the open literature. However, only few publications exist in which the question of the optimal modelling depth is discussed for homogeneously catalysed processes. Unlike these publications, we used experimental data in the present study to compare them with simulation results using different modelling depths for homogeneous reactive distillation processes. The nonequilibrium-stage model using the Maxwell–Stefan equations, the nonequilibrium-stage model using effective diffusion coefficients, the equilibrium-stage model including reaction kinetics, and the equilibrium-stage model assuming chemical equilibrium were investigated. The homogeneously catalysed transesterification of dimethyl carbonate with ethanol, for which pilot-scale experimental data were available, was used as a test system.